# Supporting Information - 2

# Structural Revision of a Wnt/β-catenin Modulator and Confirmation of Cannabielsoin Constitution and Configuration

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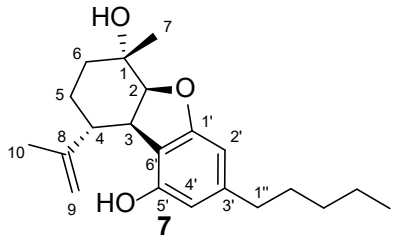
**Table of Contents**

1. Atom numbering key for DFT calculations.



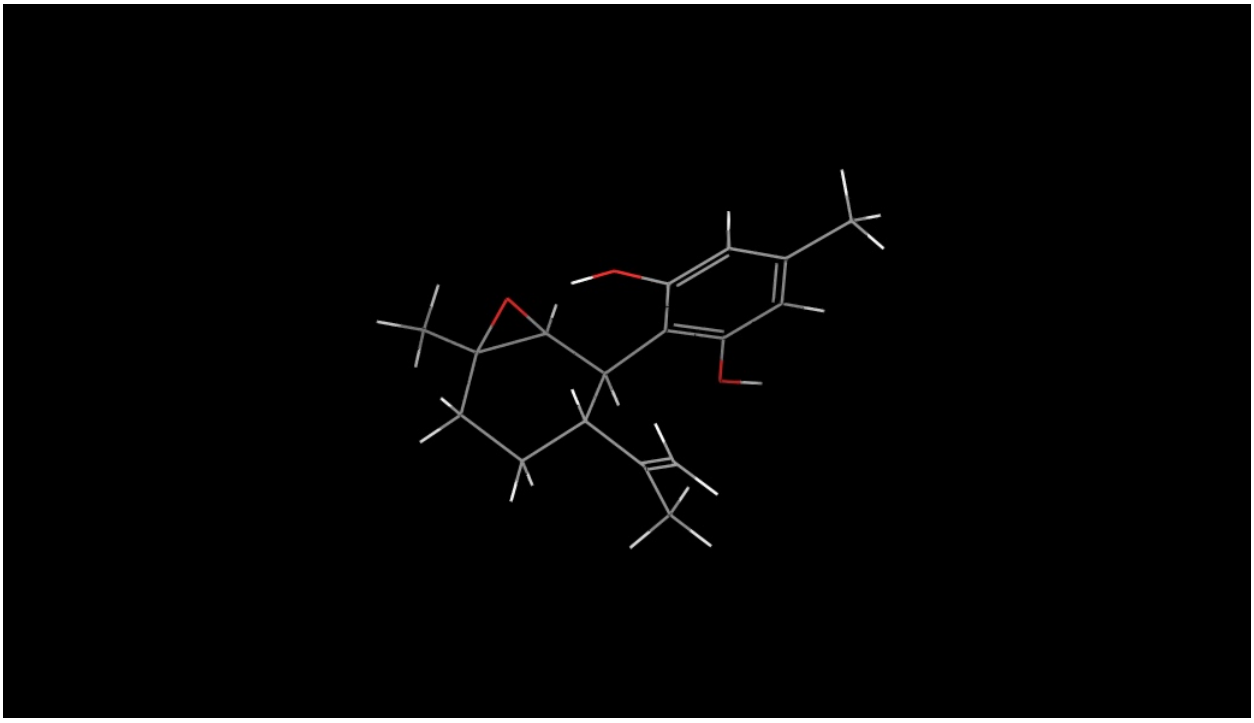
**7**

| | CBE (7) & Alternate CBE configuration at C1 (8) | 1*R*, 2*S*-CBD epoxide (5) | 6-membered cyclic ether (9) |
|---|---|---|---|
| **Literature Numbering** | **DFT numbering** | **DFT numbering** | **DFT numbering** |
| 1 | 6 | 6 | 6 |
| 2 | 5 | 5 | 5 |
| 3 | 4 | 4 | 4 |
| 4 | 3 | 3 | 3 |
| 5 | 2 | 2 | 2 |
| 6 | 1 | 1 | 1 |
| 7 | 7 | 7 | 7 |
| 8 | 8 | 14 | 8 |
| 9 | 20 | 15 | 18 |
| 10 | 19 | 16 | 19 |
| 1' | 11 | 13 | 12 |
| 2' | 9 | 8 | 9 |
| 3' | 10 | 9 | 10 |
| 4' | 14 | 10 | 15 |
| 5' | 13 | 11 | 14 |
| 6' | 12 | 12 | 13 |

2. DFT calculation data for 1*R*,2*S*-CBD epoxide (**5**). Energies, optimized geometries, NMR shielding values and IR frequencies from calculations performed at the mPW1PW91/6-311+G(2d,p)//M06-2X-D3/6-31G(d,p) level.

Conformer #1:

Boltzmann Population = 64.0% (relative energy = 0.00 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures
T = 298.15 K, P = 1.00 atm

Total internal energy, Utot (SCFE + ZPE + U): -885.956030 hartrees

Total enthalpy, Htot (Utot + pV): -885.955086 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.017416 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.451400 | -2.518800 | 0.082100 |

| | | | | | |
|---|---|---|---|---|---|
| 2 | 6 | 0 | -0.448700 | -3.555200 | 0.592600 |
| 3 | 6 | 0 | -0.557200 | -3.734500 | 2.112100 |
| 4 | 6 | 0 | -0.104300 | -2.424300 | 2.806500 |
| 5 | 6 | 0 | -0.806800 | -1.211900 | 2.228900 |
| 6 | 6 | 0 | -1.455300 | -1.238400 | 0.903800 |
| 7 | 6 | 0 | -1.647700 | 0.048200 | 0.141900 |
| 8 | 6 | 0 | -0.221300 | -2.499100 | 4.317600 |
| 9 | 6 | 0 | -1.433700 | -2.755600 | 4.979900 |
| 10 | 6 | 0 | -1.477100 | -2.931500 | 6.364200 |
| 11 | 6 | 0 | -0.321800 | -2.843600 | 7.129600 |
| 12 | 6 | 0 | 0.888200 | -2.566700 | 6.494400 |
| 13 | 6 | 0 | 0.927400 | -2.405100 | 5.113300 |
| 14 | 6 | 0 | 0.225800 | -4.925200 | 2.621500 |
| 15 | 6 | 0 | -0.392200 | -5.903500 | 3.282400 |
| 16 | 6 | 0 | 1.711800 | -4.945100 | 2.373800 |
| 17 | 8 | 0 | -2.618500 | -2.880500 | 4.332000 |
| 18 | 8 | 0 | 2.111700 | -2.149100 | 4.472300 |
| 19 | 6 | 0 | -0.370100 | -3.062500 | 8.620100 |
| 20 | 8 | 0 | -2.232900 | -1.297500 | 2.112100 |
| 21 | 1 | 0 | -1.235700 | -2.268900 | -0.961800 |
| 22 | 1 | 0 | -2.468500 | -2.927900 | 0.106300 |
| 23 | 1 | 0 | 0.568300 | -3.229100 | 0.338800 |
| 24 | 1 | 0 | -0.612600 | -4.514300 | 0.090500 |
| 25 | 1 | 0 | -1.609900 | -3.915000 | 2.356200 |
| 26 | 1 | 0 | 0.956600 | -2.280100 | 2.574200 |
| 27 | 1 | 0 | -0.461700 | -0.251600 | 2.614200 |
| 28 | 1 | 0 | -2.568300 | 0.001800 | -0.447600 |
| 29 | 1 | 0 | -1.718100 | 0.892300 | 0.830800 |
| 30 | 1 | 0 | -0.811700 | 0.215300 | -0.543100 |
| 31 | 1 | 0 | -2.441700 | -3.129400 | 6.819800 |
| 32 | 1 | 0 | 1.804400 | -2.480800 | 7.075000 |
| 33 | 1 | 0 | 0.151000 | -6.765600 | 3.658200 |
| 34 | 1 | 0 | -1.458700 | -5.861700 | 3.484100 |
| 35 | 1 | 0 | 2.202600 | -4.104400 | 2.877600 |
| 36 | 1 | 0 | 2.154300 | -5.870900 | 2.748100 |
| 37 | 1 | 0 | 1.943200 | -4.866500 | 1.305500 |
| 38 | 1 | 0 | -2.597000 | -2.441200 | 3.464900 |
| 39 | 1 | 0 | 2.822200 | -2.159400 | 5.122800 |
| 40 | 1 | 0 | -1.320200 | -2.720800 | 9.037200 |
| 41 | 1 | 0 | -0.268300 | -4.126400 | 8.857900 |
| 42 | 1 | 0 | 0.438800 | -2.530400 | 9.126800 |

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SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 155.0202 Anisotropy = 23.4671

XX= 149.6471 YX= -4.1107 ZX= 2.2065

XY= -2.6097 YY= 166.0705 ZY= -9.4789

XZ= -4.7111 YZ= -9.4909 ZZ= 149.3430

Eigenvalues: 143.9025 150.4932 170.6650

2 C Isotropic = 156.1293 Anisotropy = 16.1127

XX= 166.0654 YX= -2.3979 ZX= -0.8734

```
XY=    -4.0024   YY=   152.8028   ZY=    -0.7218
XZ=     2.0337   YZ=    -4.2623   ZZ=   149.5198
Eigenvalues:   148.1153   153.4016   166.8711
   3  C    Isotropic =   144.0710   Anisotropy =    30.4820
XX=   150.6084   YX=    13.1990   ZX=     1.0765
XY=    13.1424   YY=   151.7998   ZY=     3.7351
XZ=    -1.5018   YZ=    -2.2862   ZZ=   129.8049
Eigenvalues:   129.7490   138.0717   164.3924
   4  C    Isotropic =   147.5982   Anisotropy =    22.7020
XX=   144.8831   YX=    -2.2415   ZX=     0.1907
XY=    -9.7362   YY=   155.9236   ZY=    -7.6103
XZ=    -2.4349   YZ=   -13.0661   ZZ=   141.9878
Eigenvalues:   134.9035   145.1582   162.7329
   5  C    Isotropic =   120.5496   Anisotropy =    52.7303
XX=    93.5737   YX=    10.5193   ZX=   -18.8588
XY=    13.2411   YY=   142.9286   ZY=    -8.2412
XZ=   -20.5223   YZ=   -16.1903   ZZ=   125.1466
Eigenvalues:    83.5801   122.3655   155.7031
   6  C    Isotropic =   125.4540   Anisotropy =    55.9141
XX=    83.5120   YX=     3.1299   ZX=   -23.9139
XY=    -0.2507   YY=   156.2684   ZY=   -10.4721
XZ=   -28.5959   YZ=    -9.7661   ZZ=   136.5814
Eigenvalues:    72.6414   140.9905   162.7300
   7  C    Isotropic =   162.0615   Anisotropy =    43.5907
XX=   167.6907   YX=     8.8366   ZX=   -16.3395
XY=     8.3783   YY=   171.5261   ZY=   -20.3000
XZ=   -11.6260   YZ=   -17.9449   ZZ=   146.9677
Eigenvalues:   134.2484   160.8142   191.1220
   8  C    Isotropic =    73.4556   Anisotropy =   124.8022
XX=    26.1976   YX=    16.4827   ZX=    -0.6726
XY=    19.2686   YY=   130.5719   ZY=   -45.0002
XZ=    -8.3545   YZ=   -47.4830   ZZ=    63.5974
Eigenvalues:    22.7603    40.9495   156.6571
   9  C    Isotropic =    22.5334   Anisotropy =   140.9472
XX=   -19.7946   YX=   -11.7454   ZX=   -39.2653
XY=    -2.4838   YY=    89.0880   ZY=   -53.4928
XZ=   -41.1938   YZ=   -57.9393   ZZ=    -1.6931
Eigenvalues:   -63.8866    14.9887   116.4982
  10  C    Isotropic =    71.5417   Anisotropy =   120.0691
XX=    65.3786   YX=    13.2704   ZX=    16.1668
XY=    13.8486   YY=   116.6344   ZY=   -66.1070
XZ=    21.3046   YZ=   -62.6073   ZZ=    32.6122
Eigenvalues:    -9.2810    72.3184   151.5878
  11  C    Isotropic =    42.7669   Anisotropy =   194.2449
XX=   -50.4400   YX=    22.8163   ZX=     8.8101
XY=    21.0316   YY=   137.1072   ZY=   -66.7492
XZ=     7.5113   YZ=   -66.0163   ZZ=    41.6336
Eigenvalues:   -56.2065    12.2438   172.2635
  12  C    Isotropic =    79.7747   Anisotropy =    96.5553
XX=    54.0916   YX=   -13.0485   ZX=   -39.5934
XY=   -20.9954   YY=   126.7729   ZY=   -38.3437
XZ=   -39.5795   YZ=   -38.7994   ZZ=    58.4597
```

```
Eigenvalues:     4.0196    91.1597   144.1450
  13  C    Isotropic =    28.2724   Anisotropy =   133.0311
XX=    22.6274   YX=    18.6909   ZX=    19.3799
XY=    19.7814   YY=    76.4814   ZY=   -74.2149
XZ=    11.4818   YZ=   -69.2751   ZZ=   -14.2915
Eigenvalues:   -60.1192    27.9766   116.9599
  14  C    Isotropic =    31.1228   Anisotropy =   190.3842
XX=    95.0735   YX=   -82.5810   ZX=    19.6116
XY=   -81.5138   YY=   -21.8595   ZY=   -71.7578
XZ=    22.9483   YZ=   -68.1534   ZZ=    20.1545
Eigenvalues:   -91.5408    26.8636   158.0457
  15  C    Isotropic =    69.4797   Anisotropy =   108.1205
XX=   110.3606   YX=   -52.1131   ZX=    -6.3560
XY=   -54.3799   YY=    16.3838   ZY=   -53.3076
XZ=    -4.9252   YZ=   -55.8031   ZZ=    81.6948
Eigenvalues:   -31.8783    98.7574   141.5601
  16  C    Isotropic =   168.5390   Anisotropy =    29.0979
XX=   157.6632   YX=     1.3475   ZX=     2.7799
XY=     0.6371   YY=   173.7417   ZY=    14.5384
XZ=     1.0406   YZ=    13.0991   ZZ=   174.2122
Eigenvalues:   157.3802   160.2992   187.9376
  17  O    Isotropic =   200.4024   Anisotropy =    88.6523
XX=   157.7144   YX=     4.3193   ZX=    18.4947
XY=    17.0423   YY=   228.6846   ZY=   -60.5844
XZ=    30.4262   YZ=   -12.4557   ZZ=   214.8083
Eigenvalues:   141.8482   199.8551   259.5040
  18  O    Isotropic =   212.3209   Anisotropy =    51.8655
XX=   173.5224   YX=    -5.5411   ZX=   -10.8141
XY=    -8.0516   YY=   225.5591   ZY=     4.8230
XZ=   -27.6186   YZ=     9.7840   ZZ=   237.8813
Eigenvalues:   167.8465   222.2184   246.8980
  19  C    Isotropic =   164.4873   Anisotropy =    40.9153
XX=   190.0622   YX=   -10.7182   ZX=    -1.2732
XY=    -3.2101   YY=   147.5863   ZY=     5.5506
XZ=    -5.8804   YZ=     7.4082   ZZ=   155.8133
Eigenvalues:   143.5869   158.1108   191.7642
  20  O    Isotropic =   262.3675   Anisotropy =   135.6304
XX=   330.0888   YX=    12.2344   ZX=     4.4493
XY=    34.4647   YY=   268.6804   ZY=  -118.5916
XZ=    10.6374   YZ=   -94.2211   ZZ=   188.3332
Eigenvalues:   113.0127   321.3020   352.7877
  21  H    Isotropic =    29.9462   Anisotropy =     8.7388
XX=    35.5129   YX=    -0.1688   ZX=    -1.6868
XY=    -1.1127   YY=    29.3831   ZY=    -0.8990
XZ=    -1.3624   YZ=    -0.6596   ZZ=    24.9427
Eigenvalues:    24.5722    29.4945    35.7721
  22  H    Isotropic =    29.8767   Anisotropy =     8.0630
XX=    28.6800   YX=     1.1220   ZX=     3.6046
XY=    -0.3838   YY=    27.9985   ZY=    -0.4027
XZ=     4.1621   YZ=     0.3799   ZZ=    32.9515
Eigenvalues:    26.3213    28.0567    35.2520
  23  H    Isotropic =    30.2468   Anisotropy =     6.8914
```

```
XX=    30.5571   YX=     0.0844   ZX=    -2.0738
XY=    -0.1396   YY=    31.3696   ZY=     4.7475
XZ=    -1.2586   YZ=     3.8734   ZZ=    28.8138
Eigenvalues:    25.2605    30.6389    34.8411
  24  H    Isotropic =    30.3720   Anisotropy =     9.3929
XX=    30.8233   YX=    -1.7997   ZX=     2.3680
XY=    -2.4062   YY=    33.0978   ZY=    -3.7781
XZ=     3.1222   YZ=    -3.7417   ZZ=    27.1949
Eigenvalues:    24.8852    29.5969    36.6339
  25  H    Isotropic =    28.7616   Anisotropy =     3.4998
XX=    27.7663   YX=     0.3197   ZX=    -2.1262
XY=    -1.9274   YY=    28.6981   ZY=     0.4914
XZ=    -1.6923   YZ=    -0.1569   ZZ=    29.8203
Eigenvalues:    26.4573    28.7327    31.0948
  26  H    Isotropic =    27.8738   Anisotropy =     8.9753
XX=    28.4858   YX=     1.0396   ZX=     3.7169
XY=     1.9984   YY=    26.2582   ZY=     3.7830
XZ=     3.2369   YZ=     3.0978   ZZ=    28.8775
Eigenvalues:    23.7088    26.0553    33.8573
  27  H    Isotropic =    28.7553   Anisotropy =     9.9498
XX=    26.0672   YX=     3.6468   ZX=     0.6432
XY=     1.9921   YY=    28.9310   ZY=    -6.1323
XZ=     2.6741   YZ=    -4.1320   ZZ=    31.2677
Eigenvalues:    22.1486    28.7289    35.3885
  28  H    Isotropic =    30.1433   Anisotropy =     9.5537
XX=    32.9861   YX=     3.9251   ZX=     2.4545
XY=     5.2340   YY=    29.6093   ZY=     0.8816
XZ=     0.9528   YZ=     0.1729   ZZ=    27.8344
Eigenvalues:    26.1988    27.7186    36.5124
  29  H    Isotropic =    31.1901   Anisotropy =    10.5691
XX=    29.5485   YX=     1.0333   ZX=    -0.5830
XY=     0.9539   YY=    35.2447   ZY=    -5.2516
XZ=    -0.4863   YZ=    -5.0427   ZZ=    28.7770
Eigenvalues:    25.9321    29.4020    38.2361
  30  H    Isotropic =    30.3651   Anisotropy =    10.1904
XX=    31.8638   YX=    -0.3902   ZX=    -5.4634
XY=     1.4242   YY=    27.6488   ZY=    -0.2596
XZ=    -5.3869   YZ=     0.5064   ZZ=    31.5826
Eigenvalues:    26.1600    27.7765    37.1587
  31  H    Isotropic =    25.1770   Anisotropy =     7.4655
XX=    29.9131   YX=    -0.4550   ZX=     1.4191
XY=    -0.5419   YY=    22.4209   ZY=     1.4931
XZ=     1.1228   YZ=     1.1643   ZZ=    23.1972
Eigenvalues:    21.2656    24.1115    30.1540
  32  H    Isotropic =    25.8117   Anisotropy =     6.7535
XX=    28.6251   YX=    -2.1307   ZX=    -1.8363
XY=    -2.0729   YY=    22.9518   ZY=     1.4185
XZ=    -1.4154   YZ=     1.9438   ZZ=    25.8583
Eigenvalues:    21.9077    25.2133    30.3141
  33  H    Isotropic =    27.1777   Anisotropy =     6.4891
XX=    26.5010   YX=     1.3142   ZX=    -1.7379
XY=    -0.5086   YY=    26.6909   ZY=    -1.6307
```

```
XZ=    -3.0267   YZ=    -4.2132   ZZ=    28.3412
Eigenvalues:    23.8470    26.1823    31.5038
  34  H    Isotropic =    26.8709   Anisotropy =     7.4573
XX=    25.7598   YX=    -0.6828   ZX=    -3.4551
XY=    -0.4219   YY=    25.5803   ZY=    -4.7982
XZ=    -1.3429   YZ=    -1.9891   ZZ=    29.2727
Eigenvalues:    22.5482    26.2222    31.8425
  35  H    Isotropic =    29.5214   Anisotropy =     7.1318
XX=    26.5586   YX=    -0.7119   ZX=     4.9115
XY=    -1.6975   YY=    31.3054   ZY=     0.1114
XZ=     4.0957   YZ=    -1.9529   ZZ=    30.7001
Eigenvalues:    23.6367    30.6516    34.2759
  36  H    Isotropic =    30.3700   Anisotropy =     8.7062
XX=    28.3340   YX=     2.9604   ZX=    -1.1023
XY=     3.3966   YY=    34.8811   ZY=    -0.2028
XZ=     0.1927   YZ=     0.9518   ZZ=    27.8948
Eigenvalues:    26.7643    28.1715    36.1741
  37  H    Isotropic =    30.2509   Anisotropy =     7.6669
XX=    31.9481   YX=    -1.0827   ZX=    -1.7692
XY=    -2.4900   YY=    32.1561   ZY=     3.9249
XZ=    -1.9486   YZ=     2.4947   ZZ=    26.6486
Eigenvalues:    25.0309    30.3597    35.3622
  38  H    Isotropic =    24.4130   Anisotropy =    23.8654
XX=    36.3205   YX=     2.2986   ZX=    -8.8806
XY=     6.1974   YY=    16.0192   ZY=     4.3170
XZ=    -8.0940   YZ=     3.0650   ZZ=    20.8992
Eigenvalues:    11.3445    21.5712    40.3233
  39  H    Isotropic =    28.2131   Anisotropy =    14.4805
XX=    32.0372   YX=     0.8044   ZX=     4.5816
XY=     1.9738   YY=    22.6248   ZY=     5.2637
XZ=     6.5277   YZ=     4.5343   ZZ=    29.9772
Eigenvalues:    20.0140    26.7584    37.8667
  40  H    Isotropic =    29.6512   Anisotropy =     8.1917
XX=    30.9320   YX=    -3.3181   ZX=    -1.7108
XY=    -2.4767   YY=    30.1501   ZY=     4.3248
XZ=     0.1930   YZ=     3.7846   ZZ=    27.8715
Eigenvalues:    24.5602    29.2811    35.1124
  41  H    Isotropic =    29.3740   Anisotropy =     8.7520
XX=    31.9840   YX=     2.3430   ZX=    -2.6893
XY=     3.5290   YY=    28.1555   ZY=    -1.9871
XZ=    -3.0921   YZ=    -1.7603   ZZ=    27.9825
Eigenvalues:    26.1902    26.7232    35.2087
  42  H    Isotropic =    29.8861   Anisotropy =     8.1399
XX=    32.9129   YX=    -1.4758   ZX=     3.9109
XY=    -2.6048   YY=    25.6019   ZY=     0.2641
XZ=     1.9963   YZ=     0.6311   ZZ=    31.1436
Eigenvalues:    24.8170    29.5286    35.3128
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 51.09 | 66.40 | 82.15 | 89.04 | 117.01 | 142.49 |
| intensities | 0.21 | 0.03 | 1.49 | 0.41 | 0.51 | 0.81 |
| reduc. mass | 1.13 | 1.14 | 0.90 | 1.15 | 0.83 | 0.91 |
| force const | 0.00 | 0.00 | 0.00 | 0.01 | 0.01 | 0.01 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 179.38 | 201.00 | 239.75 | 244.10 | 254.55 | 266.86 |
| intensities | 1.79 | 0.58 | 1.96 | 0.87 | 2.96 | 1.74 |
| reduc. mass | 0.81 | 0.80 | 0.97 | 1.20 | 0.61 | 0.74 |
| force const | 0.02 | 0.02 | 0.03 | 0.04 | 0.02 | 0.03 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 275.72 | 279.82 | 315.42 | 321.20 | 334.15 | 360.98 |
| intensities | 2.45 | 0.34 | 1.63 | 0.26 | 0.42 | 10.16 |
| reduc. mass | 0.69 | 0.24 | 1.14 | 0.59 | 0.46 | 3.17 |
| force const | 0.03 | 0.01 | 0.07 | 0.04 | 0.03 | 0.24 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 370.57 | 399.67 | 445.17 | 450.35 | 494.22 | 508.89 |
| intensities | 1.14 | 1.85 | 6.70 | 4.10 | 7.69 | 13.00 |
| reduc. mass | 0.29 | 0.46 | 1.25 | 0.74 | 0.51 | 0.54 |
| force const | 0.02 | 0.04 | 0.15 | 0.09 | 0.07 | 0.08 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 520.79 | 527.65 | 529.56 | 558.99 | 592.14 | 616.94 |
| intensities | 5.50 | 7.80 | 8.41 | 8.12 | 5.25 | 26.84 |
| reduc. mass | 2.79 | 1.23 | 0.52 | 0.57 | 1.36 | 0.52 |
| force const | 0.45 | 0.20 | 0.09 | 0.10 | 0.28 | 0.12 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 631.98 | 676.29 | 700.99 | 724.33 | 727.45 | 739.22 |
| intensities | 15.94 | 2.94 | 3.68 | 19.91 | 2.78 | 23.04 |
| reduc. mass | 0.59 | 1.42 | 0.90 | 0.70 | 0.30 | 0.53 |
| force const | 0.14 | 0.38 | 0.26 | 0.21 | 0.09 | 0.17 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 757.45 | 788.50 | 812.93 | 832.46 | 889.97 | 895.96 |
| intensities | 18.80 | 9.76 | 6.24 | 5.94 | 11.92 | 6.25 |
| reduc. mass | 0.74 | 1.22 | 0.43 | 2.37 | 0.51 | 0.62 |
| force const | 0.25 | 0.45 | 0.17 | 0.97 | 0.24 | 0.29 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 934.63 | 940.57 | 956.51 | 1001.48 | 1015.71 | 1021.94 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 1.93 | 1.67 | 21.99 | 5.10 | 12.88 | 31.09 |
| reduc. mass | 1.16 | 0.58 | 0.73 | 0.30 | 0.23 | 0.30 |
| force const | 0.59 | 0.30 | 0.40 | 0.18 | 0.14 | 0.19 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1028.37 | 1041.70 | 1053.62 | 1056.58 | 1067.76 | 1096.80 |
| intensities | 32.40 | 9.33 | 8.10 | 7.64 | 7.31 | 36.55 |
| reduc. mass | 0.48 | 0.44 | 0.83 | 0.44 | 0.36 | 0.66 |
| force const | 0.30 | 0.28 | 0.55 | 0.29 | 0.24 | 0.47 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1112.51 | 1132.84 | 1137.58 | 1148.29 | 1176.81 | 1210.70 |
| intensities | 16.34 | 13.32 | 6.53 | 22.45 | 4.17 | 23.84 |
| reduc. mass | 0.45 | 0.48 | 0.36 | 0.32 | 0.37 | 0.71 |
| force const | 0.33 | 0.36 | 0.27 | 0.25 | 0.30 | 0.61 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1250.43 | 1259.68 | 1260.91 | 1264.30 | 1279.96 | 1339.24 |
| intensities | 54.94 | 65.68 | 57.36 | 19.38 | 29.59 | 2.53 |
| reduc. mass | 1.17 | 0.32 | 0.74 | 0.23 | 0.70 | 0.58 |
| force const | 1.08 | 0.30 | 0.70 | 0.22 | 0.68 | 0.61 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1356.77 | 1390.90 | 1404.04 | 1415.05 | 1460.40 | 1480.93 |
| intensities | 57.48 | 50.44 | 19.82 | 452.14 | 52.18 | 1.48 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.43 | 0.38 | 1.97 | 1.04 | 0.88 | 0.61 |
| force const | 0.47 | 0.44 | 2.29 | 1.23 | 1.11 | 0.79 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1502.04 | 1505.75 | 1515.25 | 1525.15 | 1544.86 | 1564.99 |
| intensities | 1.09 | 18.00 | 58.02 | 4.18 | 26.71 | 26.57 |
| reduc. mass | 0.79 | 1.63 | 0.87 | 2.43 | 0.66 | 0.76 |
| force const | 1.05 | 2.18 | 1.18 | 3.33 | 0.92 | 1.10 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1580.14 | 1602.34 | 1612.90 | 1635.55 | 1646.74 | 1648.27 |
| intensities | 16.10 | 8.52 | 8.45 | 9.34 | 96.35 | 32.37 |
| reduc. mass | 1.65 | 0.64 | 0.73 | 0.71 | 0.60 | 0.59 |
| force const | 2.43 | 0.96 | 1.12 | 1.11 | 0.95 | 0.94 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1657.25 | 1659.77 | 1660.65 | 1662.27 | 1663.41 | 1672.11 |
| intensities | 3.05 | 38.52 | 12.18 | 33.83 | 7.58 | 71.23 |
| reduc. mass | 0.36 | 0.20 | 0.26 | 0.13 | 0.13 | 0.75 |
| force const | 0.58 | 0.32 | 0.42 | 0.21 | 0.22 | 1.24 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1681.86 | 1682.79 | 1683.82 | 1699.50 | 1791.89 | 1819.63 |
| intensities | 14.46 | 13.21 | 11.45 | 28.54 | 865.61 | 128.68 |
| reduc. mass | 0.38 | 0.32 | 0.31 | 0.94 | 1.35 | 1.21 |
| force const | 0.64 | 0.53 | 0.52 | 1.59 | 2.55 | 2.37 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3057.41 | 3088.62 | 3095.76 | 3105.22 | 3120.99 | 3124.47 |
| intensities | 625.95 | 548.09 | 184.14 | 53.15 | 223.71 | 417.89 |
| reduc. mass | 0.48 | 0.45 | 0.46 | 0.42 | 0.85 | 0.29 |
| force const | 2.64 | 2.55 | 2.62 | 2.39 | 4.89 | 1.69 |

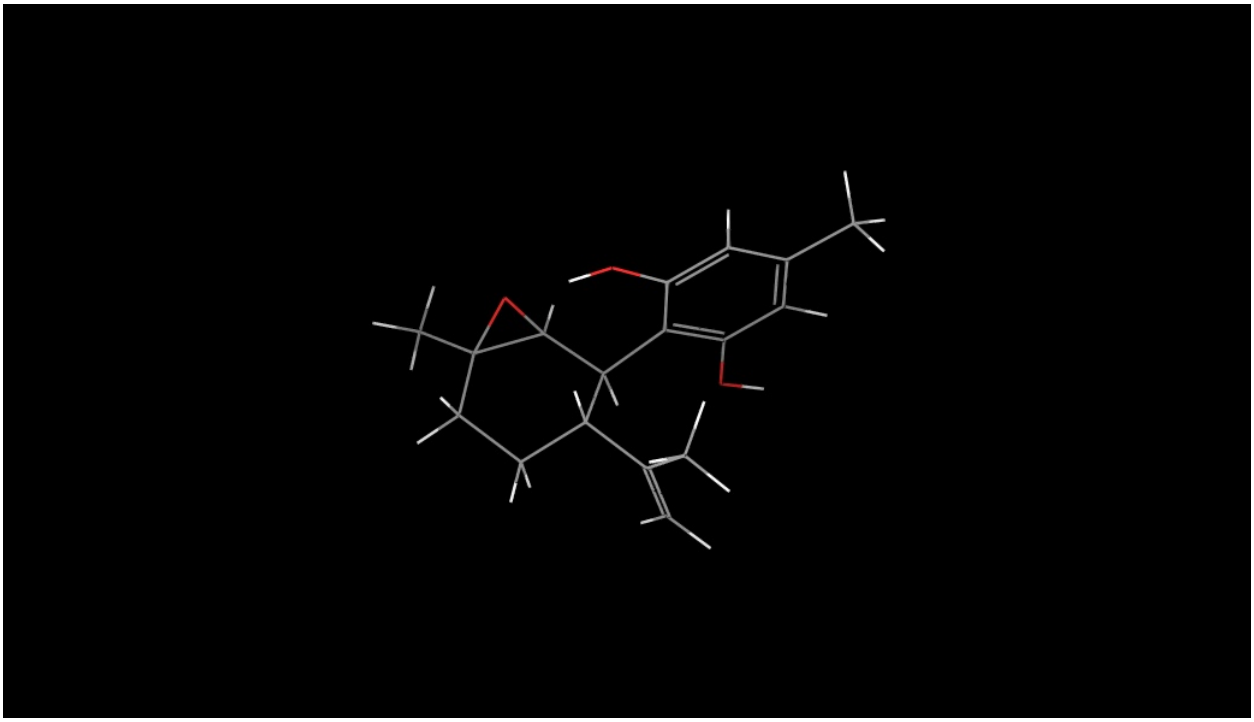
| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3128.20 | 3131.86 | 3135.10 | 3135.99 | 3138.68 | 3144.25 |
| intensities | 198.30 | 281.39 | 482.43 | 408.56 | 488.62 | 340.40 |
| reduc. mass | 0.30 | 0.48 | 0.57 | 0.35 | 0.51 | 0.55 |
| force const | 1.74 | 2.79 | 3.33 | 2.03 | 2.95 | 3.20 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3147.06 | 3149.87 | 3154.52 | 3197.46 | 3807.98 | 3858.01 |
| intensities | 335.22 | 364.91 | 388.01 | 304.05 | 522.06 | 21.90 |
| reduc. mass | 0.50 | 0.56 | 0.84 | 0.56 | 0.94 | 0.94 |
| force const | 2.89 | 3.25 | 4.93 | 3.38 | 8.03 | 8.27 |

Number of imaginary frequencies: 0

Conformation 2

Boltzmann Population = 11.1% (relative energy = 1.04 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.983588 hartrees

Total enthalpy, Htot (Utot + pV): -885.982644 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.044700 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.487300 | -2.542800 | 0.095100 |
| 2 | 6 | 0 | -0.468200 | -3.564500 | 0.601800 |
| 3 | 6 | 0 | -0.527400 | -3.720600 | 2.124100 |
| 4 | 6 | 0 | -0.107300 | -2.391300 | 2.798100 |

| | | | | | |
|---|---|---|---|---|---|
| 5 | 6 | 0 | -0.816000 | -1.191100 | 2.205600 |
| 6 | 6 | 0 | -1.475700 | -1.243500 | 0.886500 |
| 7 | 6 | 0 | -1.667100 | 0.026600 | 0.097300 |
| 8 | 6 | 0 | -0.225300 | -2.470700 | 4.309900 |
| 9 | 6 | 0 | -1.442100 | -2.705900 | 4.973400 |
| 10 | 6 | 0 | -1.482600 | -2.913100 | 6.354500 |
| 11 | 6 | 0 | -0.319300 | -2.882400 | 7.112700 |
| 12 | 6 | 0 | 0.894900 | -2.629400 | 6.476100 |
| 13 | 6 | 0 | 0.932600 | -2.432200 | 5.098800 |
| 14 | 6 | 0 | 0.338800 | -4.861900 | 2.639600 |
| 15 | 6 | 0 | 1.632500 | -4.953400 | 2.333000 |
| 16 | 6 | 0 | -0.347600 | -5.857600 | 3.533000 |
| 17 | 8 | 0 | -2.631600 | -2.796800 | 4.331000 |
| 18 | 8 | 0 | 2.115700 | -2.196400 | 4.457100 |
| 19 | 6 | 0 | -0.364200 | -3.141000 | 8.596900 |
| 20 | 8 | 0 | -2.244100 | -1.271600 | 2.101800 |
| 21 | 1 | 0 | -1.298800 | -2.317300 | -0.959600 |
| 22 | 1 | 0 | -2.502400 | -2.953600 | 0.153900 |
| 23 | 1 | 0 | 0.542000 | -3.242600 | 0.317200 |
| 24 | 1 | 0 | -0.635300 | -4.532900 | 0.120800 |
| 25 | 1 | 0 | -1.565800 | -3.938200 | 2.403700 |
| 26 | 1 | 0 | 0.954300 | -2.247600 | 2.570600 |
| 27 | 1 | 0 | -0.464800 | -0.223600 | 2.566600 |
| 28 | 1 | 0 | -0.836500 | 0.171300 | -0.599400 |
| 29 | 1 | 0 | -2.593600 | -0.027300 | -0.482400 |
| 30 | 1 | 0 | -1.724900 | 0.887200 | 0.766600 |
| 31 | 1 | 0 | -2.450000 | -3.093000 | 6.811600 |
| 32 | 1 | 0 | 1.816900 | -2.589100 | 7.052200 |
| 33 | 1 | 0 | 2.245600 | -5.764300 | 2.713700 |
| 34 | 1 | 0 | 2.130200 | -4.220000 | 1.704500 |
| 35 | 1 | 0 | 0.337300 | -6.640600 | 3.866400 |
| 36 | 1 | 0 | -0.761000 | -5.352700 | 4.414200 |
| 37 | 1 | 0 | -1.189600 | -6.328700 | 3.012400 |
| 38 | 1 | 0 | -2.600300 | -2.372400 | 3.455700 |
| 39 | 1 | 0 | 2.834200 | -2.278500 | 5.093200 |
| 40 | 1 | 0 | -1.294000 | -2.768900 | 9.033100 |
| 41 | 1 | 0 | -0.308500 | -4.214700 | 8.803700 |
| 42 | 1 | 0 | 0.472600 | -2.660600 | 9.109600 |

---

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 154.5431 Anisotropy = 23.6897

XX= 149.1821 YX= -3.0820 ZX= 2.3284

XY= -1.8514 YY= 165.8556 ZY= -9.5484

XZ= -4.8603 YZ= -9.8106 ZZ= 148.5918

Eigenvalues: 143.4248 149.8684 170.3363

2 C Isotropic = 154.7023 Anisotropy = 17.4369

XX= 165.8775 YX= 3.0864 ZX= 1.1616

XY= 0.0844 YY= 155.7853 ZY= 7.0222

XZ= 2.0558 YZ= 0.5685 ZZ= 142.4441

Eigenvalues: 141.3854 156.3945 166.3269

```
   3  C    Isotropic =   148.0979   Anisotropy =    25.7346
XX=   157.4650   YX=    12.1594   ZX=     1.5474
XY=     8.4957   YY=   151.5461   ZY=     3.8437
XZ=    -0.4733   YZ=    -3.9122   ZZ=   135.2827
Eigenvalues:   135.2627   143.7768   165.2543
   4  C    Isotropic =   143.0414   Anisotropy =    31.0439
XX=   128.7682   YX=    -1.0885   ZX=     2.8561
XY=    -3.4803   YY=   159.4335   ZY=    -7.3474
XZ=     0.7494   YZ=   -11.8490   ZZ=   140.9225
Eigenvalues:   128.4732   136.9137   163.7373
   5  C    Isotropic =   120.4369   Anisotropy =    52.7311
XX=    95.8717   YX=    12.6862   ZX=   -19.4727
XY=    14.8447   YY=   142.1558   ZY=    -7.3193
XZ=   -22.4605   YZ=   -15.0154   ZZ=   123.2831
Eigenvalues:    83.6616   122.0581   155.5910
   6  C    Isotropic =   125.3084   Anisotropy =    55.2836
XX=    84.6958   YX=     5.9201   ZX=   -25.5815
XY=     2.2799   YY=   155.9270   ZY=    -9.1697
XZ=   -30.0792   YZ=    -8.0360   ZZ=   135.3023
Eigenvalues:    72.3845   141.3765   162.1641
   7  C    Isotropic =   162.0775   Anisotropy =    43.3732
XX=   169.0468   YX=     9.2263   ZX=   -16.4626
XY=     8.8388   YY=   170.6039   ZY=   -19.7069
XZ=   -11.7058   YZ=   -17.2676   ZZ=   146.5818
Eigenvalues:   134.3779   160.8615   190.9930
   8  C    Isotropic =    73.6738   Anisotropy =   124.0127
XX=    27.1535   YX=    16.7913   ZX=    -0.6599
XY=    20.1951   YY=   127.3989   ZY=   -46.5079
XZ=    -8.4465   YZ=   -49.3459   ZZ=    66.4691
Eigenvalues:    23.1413    41.5312   156.3490
   9  C    Isotropic =    22.4989   Anisotropy =   142.1064
XX=   -20.6694   YX=   -11.1470   ZX=   -39.3548
XY=    -1.9575   YY=    87.7285   ZY=   -55.4702
XZ=   -42.0637   YZ=   -59.0197   ZZ=     0.4376
Eigenvalues:   -64.2183    14.4786   117.2365
  10  C    Isotropic =    72.3919   Anisotropy =   119.0189
XX=    66.6987   YX=    13.0571   ZX=    16.0299
XY=    13.0812   YY=   115.1183   ZY=   -66.1584
XZ=    21.1359   YZ=   -64.2524   ZZ=    35.3587
Eigenvalues:    -8.0332    73.4711   151.7378
  11  C    Isotropic =    42.4180   Anisotropy =   194.8143
XX=   -51.1760   YX=    21.4567   ZX=     9.1862
XY=    19.8202   YY=   134.1917   ZY=   -68.8933
XZ=     8.0615   YZ=   -68.6867   ZZ=    44.2384
Eigenvalues:   -56.7881    11.7479   172.2942
  12  C    Isotropic =    79.4969   Anisotropy =    96.8233
XX=    53.0970   YX=   -14.4572   ZX=   -38.7150
XY=   -22.0588   YY=   124.8666   ZY=   -39.3747
XZ=   -38.7719   YZ=   -40.6680   ZZ=    60.5272
Eigenvalues:     3.9927    90.4523   144.0458
  13  C    Isotropic =    27.6757   Anisotropy =   136.1980
XX=    20.0986   YX=    19.1606   ZX=    18.6808
```

```
XY=    18.0329   YY=    74.3447   ZY=   -76.8911
XZ=    10.5254   YZ=   -72.6766   ZZ=   -11.4161
Eigenvalues:   -60.7376    25.2904   118.4744
  14  C    Isotropic =    25.7953   Anisotropy =   197.6326
XX=    30.4457   YX=   -88.0584   ZX=    92.4401
XY=   -93.4987   YY=    31.9611   ZY=    -0.4523
XZ=    89.2397   YZ=    -7.1605   ZZ=    14.9791
Eigenvalues:   -99.8810    19.7165   157.5504
  15  C    Isotropic =    73.3089   Anisotropy =   130.6550
XX=    62.1259   YX=   -78.5403   ZX=    60.7803
XY=   -77.2128   YY=    69.8404   ZY=    15.3478
XZ=    62.6559   YZ=    20.0795   ZZ=    87.9605
Eigenvalues:   -38.6042    98.1188   160.4122
  16  C    Isotropic =   159.1094   Anisotropy =    43.0613
XX=   160.5195   YX=    13.7297   ZX=   -20.3941
XY=     8.5750   YY=   151.8521   ZY=    -5.8381
XZ=   -21.1938   YZ=    -6.8697   ZZ=   164.9567
Eigenvalues:   139.9113   149.6000   187.8170
  17  O    Isotropic =   200.0228   Anisotropy =    87.4344
XX=   158.7904   YX=     6.4725   ZX=    16.9529
XY=    19.9268   YY=   227.6703   ZY=   -58.9891
XZ=    28.2739   YZ=   -14.6298   ZZ=   213.6077
Eigenvalues:   142.2983   199.4577   258.3124
  18  O    Isotropic =   210.3252   Anisotropy =    52.0096
XX=   168.4360   YX=    -6.8039   ZX=    -9.6218
XY=    -6.7384   YY=   225.2008   ZY=     2.7507
XZ=   -29.3438   YZ=     8.2074   ZZ=   237.3387
Eigenvalues:   162.8782   223.0991   244.9983
  19  C    Isotropic =   164.4697   Anisotropy =    40.8772
XX=   190.0283   YX=   -10.4449   ZX=    -1.2216
XY=    -3.1680   YY=   147.8525   ZY=     5.7949
XZ=    -6.1563   YZ=     7.6492   ZZ=   155.5283
Eigenvalues:   143.5774   158.1105   191.7212
  20  O    Isotropic =   261.3806   Anisotropy =   137.1677
XX=   329.9343   YX=    12.6610   ZX=     3.4684
XY=    36.1068   YY=   264.5888   ZY=  -119.4448
XZ=     9.2418   YZ=   -94.6129   ZZ=   189.6185
Eigenvalues:   111.9839   319.3321   352.8257
  21  H    Isotropic =    29.9395   Anisotropy =     8.6342
XX=    35.4928   YX=    -0.3319   ZX=    -1.3458
XY=    -1.2758   YY=    29.4262   ZY=    -0.9612
XZ=    -0.9307   YZ=    -0.6820   ZZ=    24.8996
Eigenvalues:    24.6082    29.5147    35.6956
  22  H    Isotropic =    29.9392   Anisotropy =     7.8707
XX=    28.4923   YX=     1.1052   ZX=     3.3873
XY=    -0.3806   YY=    28.1305   ZY=    -0.4847
XZ=     3.9148   YZ=     0.1797   ZZ=    33.1947
Eigenvalues:    26.4119    28.2193    35.1863
  23  H    Isotropic =    30.2846   Anisotropy =     7.2158
XX=    30.4832   YX=    -0.1063   ZX=    -1.7619
XY=    -0.6198   YY=    31.3226   ZY=     5.0907
XZ=    -1.0641   YZ=     3.8562   ZZ=    29.0480
```

```
Eigenvalues:    25.4081    30.3507    35.0952
  24  H    Isotropic =    30.2757   Anisotropy =     9.1967
XX=    30.5345   YX=    -1.5513   ZX=     2.0271
XY=    -2.4268   YY=    32.9575   ZY=    -4.0228
XZ=     2.8612   YZ=    -3.7780   ZZ=    27.3353
Eigenvalues:    24.9960    29.4244    36.4069
  25  H    Isotropic =    29.2424   Anisotropy =     4.0883
XX=    28.7290   YX=     0.7744   ZX=    -2.4832
XY=    -1.6762   YY=    28.8673   ZY=     0.0142
XZ=    -2.3789   YZ=    -0.3052   ZZ=    30.1310
Eigenvalues:    26.8026    28.9568    31.9680
  26  H    Isotropic =    27.9745   Anisotropy =     8.7824
XX=    29.1382   YX=     0.7803   ZX=     3.5071
XY=     2.0739   YY=    25.6855   ZY=     3.6305
XZ=     3.1135   YZ=     2.9474   ZZ=    29.0999
Eigenvalues:    23.6216    26.4725    33.8294
  27  H    Isotropic =    28.8221   Anisotropy =     9.9960
XX=    26.1392   YX=     3.7778   ZX=     0.2589
XY=     2.1594   YY=    28.8105   ZY=    -6.0123
XZ=     2.2256   YZ=    -4.1169   ZZ=    31.5167
Eigenvalues:    22.3391    28.6412    35.4862
  28  H    Isotropic =    30.3385   Anisotropy =    10.1725
XX=    32.1177   YX=    -0.6257   ZX=    -5.4572
XY=     1.2181   YY=    27.6123   ZY=     0.0057
XZ=    -5.3476   YZ=     0.7433   ZZ=    31.2857
Eigenvalues:    26.1303    27.7651    37.1202
  29  H    Isotropic =    30.1428   Anisotropy =     9.5054
XX=    33.2117   YX=     3.7797   ZX=     2.5734
XY=     5.0630   YY=    29.2812   ZY=     0.8910
XZ=     1.0575   YZ=     0.2531   ZZ=    27.9355
Eigenvalues:    26.2192    27.7294    36.4797
  30  H    Isotropic =    31.1716   Anisotropy =    10.5869
XX=    29.6339   YX=     1.3332   ZX=    -0.7774
XY=     1.2743   YY=    35.0729   ZY=    -5.2716
XZ=    -0.6715   YZ=    -5.0341   ZZ=    28.8078
Eigenvalues:    25.9100    29.3751    38.2295
  31  H    Isotropic =    25.1818   Anisotropy =     7.3786
XX=    29.8692   YX=    -0.4235   ZX=     1.4152
XY=    -0.5358   YY=    22.6214   ZY=     1.5795
XZ=     1.0990   YZ=     1.2218   ZZ=    23.0547
Eigenvalues:    21.2558    24.1887    30.1008
  32  H    Isotropic =    25.8307   Anisotropy =     6.6402
XX=    28.5649   YX=    -2.1840   ZX=    -1.7610
XY=    -2.0755   YY=    23.0248   ZY=     1.5897
XZ=    -1.2880   YZ=     1.9432   ZZ=    25.9025
Eigenvalues:    21.8969    25.3378    30.2576
  33  H    Isotropic =    26.7623   Anisotropy =     5.7842
XX=    24.4644   YX=    -1.3670   ZX=    -0.1413
XY=    -0.2842   YY=    29.1010   ZY=     1.4773
XZ=     1.7726   YZ=     3.3587   ZZ=    26.7214
Eigenvalues:    23.6438    26.0247    30.6184
  34  H    Isotropic =    26.6817   Anisotropy =     8.4486
```

```
XX=    24.4875   YX=     0.5330   ZX=     2.7766
XY=    -1.9582   YY=    29.5415   ZY=     6.1471
XZ=     0.6863   YZ=     2.1722   ZZ=    26.0162
Eigenvalues:    21.9333    25.7977    32.3141
  35  H    Isotropic =    30.5102   Anisotropy =     8.7874
XX=    29.7682   YX=     4.7328   ZX=    -1.1414
XY=     2.8461   YY=    33.2347   ZY=    -0.6913
XZ=    -2.2488   YZ=    -2.6893   ZZ=    28.5276
Eigenvalues:    27.0302    28.1319    36.3684
  36  H    Isotropic =    30.5779   Anisotropy =     7.5773
XX=    30.1383   YX=    -2.6425   ZX=    -3.2037
XY=    -3.7041   YY=    33.4126   ZY=    -3.7726
XZ=    -1.3467   YZ=    -2.0135   ZZ=    28.1826
Eigenvalues:    24.6668    31.4374    35.6294
  37  H    Isotropic =    30.2700   Anisotropy =     8.2432
XX=    27.8462   YX=     0.5048   ZX=     0.5727
XY=     0.2001   YY=    28.3923   ZY=    -3.5373
XZ=     1.5303   YZ=    -2.1266   ZZ=    34.5715
Eigenvalues:    26.7795    28.2650    35.7655
  38  H    Isotropic =    24.1146   Anisotropy =    24.8633
XX=    36.9590   YX=     1.8847   ZX=    -8.9471
XY=     5.4182   YY=    15.3178   ZY=     4.5723
XZ=    -8.1978   YZ=     3.2135   ZZ=    20.0670
Eigenvalues:    10.7983    20.8554    40.6901
  39  H    Isotropic =    28.2608   Anisotropy =    14.4040
XX=    31.9963   YX=     1.2833   ZX=     4.4188
XY=     2.5010   YY=    23.2273   ZY=     5.8724
XZ=     6.1674   YZ=     4.7855   ZZ=    29.5588
Eigenvalues:    20.0944    26.8245    37.8634
  40  H    Isotropic =    29.6237   Anisotropy =     8.2105
XX=    30.8838   YX=    -3.3539   ZX=    -1.6289
XY=    -2.4900   YY=    30.3892   ZY=     4.2391
XZ=     0.2514   YZ=     3.7076   ZZ=    27.5980
Eigenvalues:    24.5486    29.2250    35.0974
  41  H    Isotropic =    29.3600   Anisotropy =     8.6736
XX=    31.9136   YX=     2.1937   ZX=    -2.7563
XY=     3.3662   YY=    28.0236   ZY=    -2.0778
XZ=    -3.1574   YZ=    -1.8371   ZZ=    28.1426
Eigenvalues:    26.1223    26.8152    35.1424
  42  H    Isotropic =    29.8704   Anisotropy =     8.1445
XX=    32.9584   YX=    -1.3138   ZX=     3.9490
XY=    -2.4800   YY=    25.6042   ZY=     0.4800
XZ=     2.0615   YZ=     0.8001   ZZ=    31.0487
Eigenvalues:    24.8124    29.4988    35.3001
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 59.14 | 87.68 | 94.71 | 109.12 | 126.58 | 138.04 |
| intensities | 0.61 | 0.25 | 1.41 | 0.83 | 0.79 | 3.02 |
| reduc. mass | 1.40 | 0.84 | 1.09 | 1.32 | 0.28 | 1.29 |
| force const | 0.00 | 0.00 | 0.01 | 0.01 | 0.00 | 0.01 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 165.66 | 192.76 | 222.97 | 246.86 | 253.37 | 266.47 |
| intensities | 0.69 | 0.55 | 1.10 | 0.95 | 6.21 | 6.14 |
| reduc. mass | 0.73 | 0.76 | 1.48 | 0.68 | 0.71 | 1.31 |
| force const | 0.01 | 0.02 | 0.04 | 0.02 | 0.03 | 0.05 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 268.27 | 294.19 | 298.92 | 305.26 | 314.60 | 343.16 |
| intensities | 0.58 | 3.40 | 1.43 | 0.96 | 0.27 | 7.97 |
| reduc. mass | 0.89 | 0.27 | 1.24 | 0.32 | 0.30 | 1.35 |
| force const | 0.04 | 0.01 | 0.07 | 0.02 | 0.02 | 0.09 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 354.19 | 401.20 | 420.57 | 450.34 | 470.29 | 495.73 |
| intensities | 4.34 | 1.78 | 6.41 | 2.54 | 20.86 | 10.94 |
| reduc. mass | 0.77 | 0.55 | 0.49 | 0.68 | 0.51 | 0.79 |
| force const | 0.06 | 0.05 | 0.05 | 0.08 | 0.07 | 0.11 |
| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 520.48 | 524.23 | 543.65 | 556.16 | 565.43 | 602.39 |
| intensities | 8.82 | 13.83 | 3.00 | 23.71 | 43.32 | 25.99 |
| reduc. mass | 0.47 | 2.09 | 0.53 | 0.56 | 0.49 | 2.16 |
| force const | 0.08 | 0.34 | 0.09 | 0.10 | 0.09 | 0.46 |

| | | | | | | |
|---|---|---|---|---|---|---|
| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 649.40 | 664.05 | 691.94 | 706.41 | 709.52 | 717.73 |
| intensities | 79.81 | 29.64 | 9.15 | 5.34 | 15.29 | 3.07 |
| reduc. mass | 0.49 | 0.76 | 1.11 | 0.82 | 0.91 | 0.36 |
| force const | 0.12 | 0.20 | 0.31 | 0.24 | 0.27 | 0.11 |

| | | | | | | |
|---|---|---|---|---|---|---|
| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 746.37 | 807.49 | 819.33 | 851.15 | 872.10 | 932.41 |
| intensities | 16.03 | 1.86 | 4.63 | 6.03 | 12.20 | 3.30 |
| reduc. mass | 0.73 | 0.99 | 1.84 | 0.75 | 0.61 | 0.75 |
| force const | 0.24 | 0.38 | 0.73 | 0.32 | 0.27 | 0.39 |

| | | | | | | |
|---|---|---|---|---|---|---|
| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 938.22 | 951.95 | 956.96 | 988.32 | 1010.25 | 1016.16 |
| intensities | 3.48 | 23.22 | 16.52 | 9.79 | 0.43 | 14.85 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.45 | 0.98 | 0.31 | 0.30 | 0.22 | 0.28 |
| force const | 0.24 | 0.52 | 0.17 | 0.17 | 0.13 | 0.17 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1030.16 | 1046.38 | 1050.01 | 1054.22 | 1056.75 | 1093.60 |
| intensities | 23.64 | 2.86 | 24.94 | 4.21 | 33.93 | 8.92 |
| reduc. mass | 0.50 | 0.55 | 0.34 | 0.26 | 0.31 | 0.60 |
| force const | 0.31 | 0.35 | 0.22 | 0.17 | 0.20 | 0.43 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1113.28 | 1132.88 | 1143.29 | 1153.81 | 1164.77 | 1210.00 |
| intensities | 28.74 | 8.16 | 6.58 | 53.68 | 54.09 | 14.54 |
| reduc. mass | 0.39 | 0.56 | 0.44 | 0.71 | 0.36 | 0.32 |
| force const | 0.29 | 0.42 | 0.34 | 0.56 | 0.28 | 0.28 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1215.04 | 1228.28 | 1253.56 | 1259.29 | 1305.87 | 1321.46 |
| intensities | 108.41 | 27.30 | 65.38 | 51.58 | 43.68 | 90.20 |
| reduc. mass | 1.20 | 0.56 | 0.40 | 0.37 | 0.67 | 0.53 |
| force const | 1.04 | 0.49 | 0.37 | 0.35 | 0.67 | 0.54 |
| H42 Z | -0.01265 | 0.01193 | -0.00183 | 0.01660 | -0.13758 | 0.01403 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1366.62 | 1400.37 | 1401.62 | 1422.62 | 1435.28 | 1484.26 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 24.04 | 215.51 | 146.05 | 201.90 | 88.15 | 10.81 |
| reduc. mass | 0.51 | 0.44 | 0.30 | 1.15 | 0.52 | 1.44 |
| force const | 0.56 | 0.51 | 0.35 | 1.37 | 0.63 | 1.87 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1497.21 | 1505.56 | 1512.09 | 1513.98 | 1526.13 | 1531.11 |
| intensities | 7.14 | 29.86 | 77.59 | 82.28 | 23.13 | 59.43 |
| reduc. mass | 0.62 | 0.64 | 1.00 | 0.86 | 0.94 | 0.72 |
| force const | 0.82 | 0.85 | 1.35 | 1.16 | 1.29 | 1.00 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1540.40 | 1566.52 | 1587.60 | 1617.72 | 1629.26 | 1632.44 |
| intensities | 36.95 | 120.02 | 18.07 | 57.25 | 50.98 | 53.63 |
| reduc. mass | 0.57 | 0.97 | 0.52 | 0.26 | 0.23 | 0.38 |
| force const | 0.79 | 1.41 | 0.78 | 0.40 | 0.35 | 0.60 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1641.26 | 1649.60 | 1656.06 | 1658.48 | 1660.43 | 1665.29 |
| intensities | 6.60 | 29.31 | 33.09 | 72.18 | 12.61 | 2.85 |
| reduc. mass | 0.52 | 1.04 | 0.13 | 0.37 | 0.34 | 0.35 |
| force const | 0.83 | 1.67 | 0.20 | 0.60 | 0.56 | 0.57 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1669.60 | 1670.15 | 1672.21 | 1687.26 | 1687.79 | 1803.55 |
| intensities | 18.74 | 6.85 | 14.40 | 78.99 | 24.19 | 854.83 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.13 | 0.27 | 0.24 | 0.55 | 0.38 | 1.63 |
| force const | 0.21 | 0.44 | 0.40 | 0.93 | 0.64 | 3.12 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1834.94 | 1889.25 | 3019.05 | 3023.29 | 3028.79 | 3049.45 |
| intensities | 370.85 | 20.27 | 233.88 | 490.19 | 587.60 | 564.50 |
| reduc. mass | 1.35 | 0.87 | 0.30 | 0.31 | 0.31 | 0.45 |
| force const | 2.68 | 1.83 | 1.63 | 1.67 | 1.67 | 2.47 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3057.36 | 3076.42 | 3077.12 | 3104.37 | 3106.12 | 3117.91 |
| intensities | 738.73 | 340.33 | 155.88 | 386.97 | 80.28 | 507.92 |
| reduc. mass | 0.42 | 0.83 | 0.68 | 0.35 | 0.27 | 0.44 |
| force const | 2.32 | 4.64 | 3.80 | 1.97 | 1.52 | 2.53 |

| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3125.57 | 3130.48 | 3135.57 | 3138.04 | 3145.35 | 3148.29 |
| intensities | 386.03 | 135.46 | 447.48 | 628.84 | 575.20 | 78.91 |
| reduc. mass | 0.47 | 0.43 | 0.46 | 0.47 | 0.29 | 0.26 |
| force const | 2.69 | 2.48 | 2.69 | 2.72 | 1.67 | 1.53 |

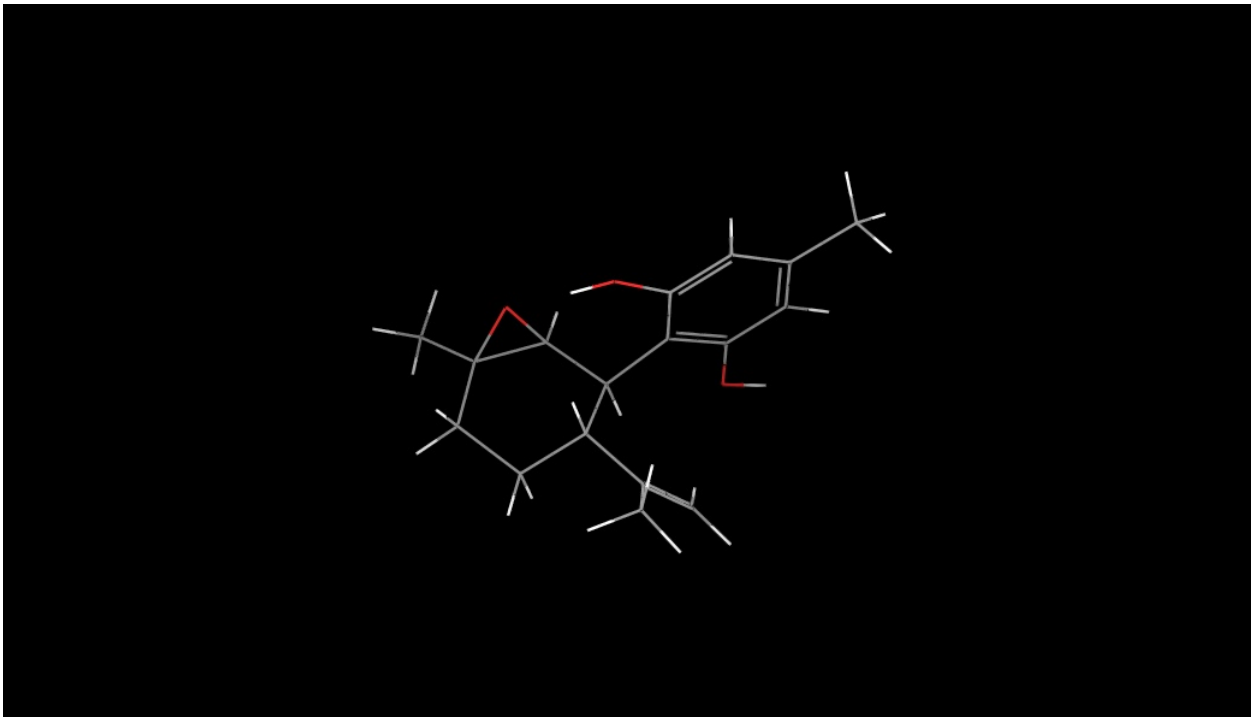
| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3152.63 | 3154.56 | 3164.94 | 3195.81 | 3826.30 | 3851.07 |
| intensities | 172.89 | 554.20 | 120.91 | 330.36 | 78.65 | 131.86 |
| reduc. mass | 0.35 | 0.48 | 0.59 | 0.56 | 0.95 | 0.95 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| force const | | 2.06 | 2.79 | 3.48 | 3.36 | 8.15 | 8.26 |
| C1 | X | 0.00075 | 0.00047 | 0.00151 | -0.00003 | -0.00030 | -0.00002 |
| C1 | Y | 0.00028 | 0.00092 | -0.00481 | -0.00052 | 0.00002 | -0.00007 |

Number of imaginary frequencies: 0

Conformation 3

Boltzmann Population = 21.3% (relative energy = 0.65 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot (SCFE + ZPE + U): -885.954634 hartrees

Total enthalpy, Htot (Utot + pV): -885.953690 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.015730 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.399900 | -2.489200 | 0.087300 |
| 2 | 6 | 0 | -0.402400 | -3.531000 | 0.594800 |
| 3 | 6 | 0 | -0.500400 | -3.733500 | 2.115300 |
| 4 | 6 | 0 | -0.069100 | -2.433300 | 2.827300 |
| 5 | 6 | 0 | -0.772400 | -1.217300 | 2.256300 |
| 6 | 6 | 0 | -1.415400 | -1.223400 | 0.928900 |

| | | | | | |
|---|---|---|---|---|---|
| 7 | 6 | 0 | -1.611100 | 0.075200 | 0.188900 |
| 8 | 6 | 0 | -0.214800 | -2.504400 | 4.337900 |
| 9 | 6 | 0 | -1.432600 | -2.788200 | 4.978400 |
| 10 | 6 | 0 | -1.498600 | -2.953600 | 6.363500 |
| 11 | 6 | 0 | -0.363700 | -2.816800 | 7.151600 |
| 12 | 6 | 0 | 0.847100 | -2.494700 | 6.539000 |
| 13 | 6 | 0 | 0.909300 | -2.343700 | 5.157700 |
| 14 | 6 | 0 | 0.293100 | -4.957500 | 2.533000 |
| 15 | 6 | 0 | 1.559200 | -4.916700 | 2.946800 |
| 16 | 6 | 0 | -0.461000 | -6.256100 | 2.419800 |
| 17 | 8 | 0 | -2.602200 | -2.947400 | 4.308200 |
| 18 | 8 | 0 | 2.091100 | -2.029700 | 4.540100 |
| 19 | 6 | 0 | -0.433100 | -3.026700 | 8.642500 |
| 20 | 8 | 0 | -2.197900 | -1.308600 | 2.132600 |
| 21 | 1 | 0 | -1.168600 | -2.223100 | -0.949300 |
| 22 | 1 | 0 | -2.417200 | -2.898900 | 0.089800 |
| 23 | 1 | 0 | 0.622100 | -3.213900 | 0.361600 |
| 24 | 1 | 0 | -0.562600 | -4.480200 | 0.073300 |
| 25 | 1 | 0 | -1.550900 | -3.934400 | 2.359300 |
| 26 | 1 | 0 | 0.993100 | -2.275600 | 2.612300 |
| 27 | 1 | 0 | -0.434300 | -0.261900 | 2.659700 |
| 28 | 1 | 0 | -0.771800 | 0.259400 | -0.487700 |
| 29 | 1 | 0 | -2.527800 | 0.034100 | -0.407100 |
| 30 | 1 | 0 | -1.690700 | 0.906400 | 0.892400 |
| 31 | 1 | 0 | -2.465600 | -3.178000 | 6.801300 |
| 32 | 1 | 0 | 1.745600 | -2.362400 | 7.138300 |
| 33 | 1 | 0 | 2.085300 | -5.833000 | 3.198100 |
| 34 | 1 | 0 | 2.105500 | -3.988500 | 3.079500 |
| 35 | 1 | 0 | 0.185100 | -7.116100 | 2.608200 |
| 36 | 1 | 0 | -1.283900 | -6.274200 | 3.143600 |
| 37 | 1 | 0 | -0.910100 | -6.373500 | 1.426700 |
| 38 | 1 | 0 | -2.581300 | -2.486100 | 3.452100 |
| 39 | 1 | 0 | 2.790100 | -2.012100 | 5.202800 |
| 40 | 1 | 0 | -1.409100 | -2.733600 | 9.036200 |
| 41 | 1 | 0 | -0.279000 | -4.081700 | 8.891500 |
| 42 | 1 | 0 | 0.334800 | -2.447800 | 9.161500 |

---

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 154.5238 Anisotropy = 22.9744
XX= 149.4141 YX= -4.5724 ZX= 1.4773
XY= -2.2635 YY= 168.0487 ZY= -5.1151
XZ= -4.6663 YZ= -6.1496 ZZ= 146.1087
Eigenvalues: 143.7146 150.0167 169.8401

2 C Isotropic = 153.4411 Anisotropy = 19.9031
XX= 165.9457 YX= 6.3524 ZX= -4.1831
XY= -1.1055 YY= 145.2294 ZY= 9.1815
XZ= -2.7494 YZ= 5.0478 ZZ= 149.1481
Eigenvalues: 139.1526 154.4609 166.7098

3 C Isotropic = 146.3161 Anisotropy = 24.1424
XX= 149.5996 YX= 11.1786 ZX= -1.0218

```
XY=     4.8369   YY=   157.2196   ZY=    -0.3507
XZ=    -4.4618   YZ=    -0.9246   ZZ=   132.1290
Eigenvalues:   131.6934   144.8438   162.4110
   4  C    Isotropic =   148.6213   Anisotropy =    20.7788
XX=   147.6038   YX=    -0.4179   ZX=    -0.1826
XY=   -10.7451   YY=   159.4551   ZY=    -2.7747
XZ=    -4.2796   YZ=    -8.1849   ZZ=   138.8048
Eigenvalues:   136.2521   147.1379   162.4738
   5  C    Isotropic =   119.7354   Anisotropy =    52.5392
XX=    91.5268   YX=    11.0391   ZX=   -15.3115
XY=    14.8845   YY=   147.1315   ZY=    -5.1174
XZ=   -16.2491   YZ=   -12.9544   ZZ=   120.5480
Eigenvalues:    83.4603   120.9845   154.7616
   6  C    Isotropic =   125.3981   Anisotropy =    55.5357
XX=    81.9890   YX=     3.8227   ZX=   -21.3866
XY=     1.3754   YY=   159.6971   ZY=    -6.8667
XZ=   -26.4606   YZ=    -6.4091   ZZ=   134.5081
Eigenvalues:    72.7252   141.0471   162.4219
   7  C    Isotropic =   162.2278   Anisotropy =    43.3292
XX=   166.2369   YX=    11.1103   ZX=   -14.2177
XY=     9.5178   YY=   178.7878   ZY=   -14.9923
XZ=    -9.8882   YZ=   -12.4889   ZZ=   141.6588
Eigenvalues:   134.6949   160.8746   191.1140
   8  C    Isotropic =    72.7359   Anisotropy =   125.0285
XX=    25.2708   YX=    15.3799   ZX=     2.5186
XY=    16.8949   YY=   146.7202   ZY=   -27.1918
XZ=    -3.0906   YZ=   -29.6779   ZZ=    46.2166
Eigenvalues:    22.4995    39.6199   156.0882
   9  C    Isotropic =    22.6122   Anisotropy =   140.0143
XX=   -20.9173   YX=    -6.4704   ZX=   -40.3764
XY=     2.9272   YY=   107.4975   ZY=   -30.4129
XZ=   -39.5238   YZ=   -35.0503   ZZ=   -18.7435
Eigenvalues:   -63.3168    15.1984   115.9551
  10  C    Isotropic =    71.5020   Anisotropy =   119.4901
XX=    66.5743   YX=     7.8677   ZX=    18.5221
XY=     7.5407   YY=   139.7253   ZY=   -42.4884
XZ=    23.2532   YZ=   -38.2388   ZZ=     8.2062
Eigenvalues:    -9.6573    73.0012   151.1620
  11  C    Isotropic =    42.9384   Anisotropy =   193.7627
XX=   -50.2916   YX=    16.6511   ZX=    15.0008
XY=    15.5963   YY=   161.4513   ZY=   -39.9503
XZ=    13.6780   YZ=   -38.4845   ZZ=    17.6554
Eigenvalues:   -55.9583    12.6598   172.1135
  12  C    Isotropic =    79.6704   Anisotropy =    96.7621
XX=    52.6194   YX=    -4.9850   ZX=   -41.1011
XY=   -12.0725   YY=   140.3914   ZY=   -18.3503
XZ=   -43.5086   YZ=   -20.2111   ZZ=    46.0004
Eigenvalues:     3.9486    90.8841   144.1785
  13  C    Isotropic =    27.7946   Anisotropy =   134.2879
XX=    22.6659   YX=    12.5870   ZX=    23.5690
XY=    15.3933   YY=   105.1947   ZY=   -44.8856
XZ=    15.0615   YZ=   -40.5141   ZZ=   -44.4766
```

```
Eigenvalues:   -61.7017    27.7657   117.3199
  14  C    Isotropic =    30.6458   Anisotropy =   188.8555
XX=   117.1530   YX=   -62.3806   ZX=   -26.9580
XY=   -63.3777   YY=   -36.0698   ZY=    72.0474
XZ=   -23.3750   YZ=    66.3301   ZZ=    10.8543
Eigenvalues:   -92.7088    28.0968   156.5495
  15  C    Isotropic =    73.9798   Anisotropy =   127.1560
XX=   128.6352   YX=   -55.5968   ZX=    -9.0490
XY=   -46.6972   YY=    11.3488   ZY=    56.4850
XZ=    -5.1658   YZ=    54.2396   ZZ=    81.9554
Eigenvalues:   -30.2820    93.4709   158.7505
  16  C    Isotropic =   161.3470   Anisotropy =    41.6982
XX=   140.1941   YX=     2.4059   ZX=     1.0294
XY=     4.4394   YY=   170.7421   ZY=   -15.7626
XZ=     1.4457   YZ=   -18.5164   ZZ=   173.1049
Eigenvalues:   139.4219   155.4734   189.1458
  17  O    Isotropic =   202.2467   Anisotropy =    85.9624
XX=   163.4849   YX=    -0.5405   ZX=    21.0560
XY=     5.9440   YY=   243.3336   ZY=   -55.0922
XZ=    32.5052   YZ=    -4.4579   ZZ=   199.9215
Eigenvalues:   146.2816   200.9034   259.5549
  18  O    Isotropic =   210.9161   Anisotropy =    51.4745
XX=   169.7169   YX=    -4.3290   ZX=    -8.6052
XY=    -2.1282   YY=   223.3469   ZY=     2.8593
XZ=   -28.0441   YZ=     5.3616   ZZ=   239.6845
Eigenvalues:   165.1282   222.3877   245.2325
  19  C    Isotropic =   164.4582   Anisotropy =    40.8819
XX=   189.9241   YX=    -9.4767   ZX=    -4.5813
XY=    -0.9989   YY=   144.8947   ZY=     2.8003
XZ=    -7.1066   YZ=     5.0583   ZZ=   158.5559
Eigenvalues:   143.5539   158.1080   191.7128
  20  O    Isotropic =   263.0820   Anisotropy =   135.3168
XX=   328.8567   YX=    10.6952   ZX=     7.7624
XY=    30.2267   YY=   308.4275   ZY=   -96.9877
XZ=    15.7417   YZ=   -70.0275   ZZ=   151.9619
Eigenvalues:   114.0927   321.8602   353.2933
  21  H    Isotropic =    29.9271   Anisotropy =     8.7488
XX=    35.4038   YX=     0.3931   ZX=    -1.9501
XY=    -0.6437   YY=    29.5111   ZY=    -0.2416
XZ=    -1.9799   YZ=    -0.1109   ZZ=    24.8665
Eigenvalues:    24.5044    29.5174    35.7596
  22  H    Isotropic =    29.8953   Anisotropy =     7.8428
XX=    28.8528   YX=     0.4063   ZX=     3.9963
XY=    -0.9912   YY=    28.5094   ZY=    -1.1625
XZ=     4.1215   YZ=    -0.5966   ZZ=    32.3235
Eigenvalues:    26.1484    28.4136    35.1238
  23  H    Isotropic =    30.7502   Anisotropy =     7.0747
XX=    30.7062   YX=    -0.1198   ZX=    -2.3389
XY=    -0.6221   YY=    29.8120   ZY=     4.5571
XZ=    -2.0279   YZ=     2.9446   ZZ=    31.7325
Eigenvalues:    26.5994    30.1846    35.4667
  24  H    Isotropic =    30.0302   Anisotropy =     8.4797
```

```
XX=    31.1102   YX=    -1.5659   ZX=     1.5237
XY=    -2.4748   YY=    33.6659   ZY=    -2.8557
XZ=     0.8948   YZ=    -2.8000   ZZ=    25.3144
Eigenvalues:    24.3958    30.0115    35.6833
  25  H    Isotropic =    28.9595   Anisotropy =     3.5981
XX=    26.2904   YX=    -0.9796   ZX=    -2.7538
XY=    -2.1318   YY=    30.3281   ZY=    -0.3946
XZ=    -1.8579   YZ=    -0.6912   ZZ=    30.2599
Eigenvalues:    24.7501    30.7701    31.3582
  26  H    Isotropic =    27.7968   Anisotropy =     9.2870
XX=    28.8762   YX=     0.8366   ZX=     3.3469
XY=     1.6443   YY=    24.2333   ZY=     3.0239
XZ=     3.7837   YZ=     2.0396   ZZ=    30.2809
Eigenvalues:    23.3126    26.0896    33.9881
  27  H    Isotropic =    28.7148   Anisotropy =     9.7586
XX=    26.1106   YX=     3.2279   ZX=     1.8063
XY=     1.1992   YY=    30.9095   ZY=    -6.1529
XZ=     3.3998   YZ=    -4.1000   ZZ=    29.1243
Eigenvalues:    21.9840    28.9398    35.2205
  28  H    Isotropic =    30.3652   Anisotropy =    10.2143
XX=    31.5081   YX=     0.8746   ZX=    -5.3615
XY=     2.5296   YY=    27.8364   ZY=    -1.3750
XZ=    -4.9651   YZ=    -0.5615   ZZ=    31.7510
Eigenvalues:    26.2338    27.6870    37.1747
  29  H    Isotropic =    30.1547   Anisotropy =     9.5255
XX=    32.7422   YX=     3.5495   ZX=     3.0365
XY=     5.0935   YY=    29.7178   ZY=     1.1415
XZ=     1.8101   YZ=     0.4083   ZZ=    28.0040
Eigenvalues:    26.1677    27.7913    36.5050
  30  H    Isotropic =    31.1738   Anisotropy =    10.5594
XX=    29.4808   YX=     0.7229   ZX=    -0.2269
XY=     0.5802   YY=    36.9897   ZY=    -3.7109
XZ=    -0.1517   YZ=    -3.5031   ZZ=    27.0509
Eigenvalues:    25.8797    29.4283    38.2134
  31  H    Isotropic =    25.2188   Anisotropy =     7.4846
XX=    30.0249   YX=    -0.5795   ZX=     1.1634
XY=    -0.6600   YY=    21.8861   ZY=     1.1544
XZ=     0.8540   YZ=     0.8642   ZZ=    23.7454
Eigenvalues:    21.3327    24.1152    30.2085
  32  H    Isotropic =    25.8029   Anisotropy =     6.7903
XX=    28.6159   YX=    -1.5523   ZX=    -2.2879
XY=    -1.4308   YY=    22.2606   ZY=     0.6332
XZ=    -1.9784   YZ=     1.2171   ZZ=    26.5322
Eigenvalues:    21.8789    25.2001    30.3298
  33  H    Isotropic =    26.9255   Anisotropy =     4.7707
XX=    25.9221   YX=     0.4995   ZX=     1.4354
XY=    -0.3489   YY=    27.4809   ZY=     1.1635
XZ=     2.8668   YZ=     2.8905   ZZ=    27.3736
Eigenvalues:    23.9521    26.7185    30.1060
  34  H    Isotropic =    26.2310   Anisotropy =     6.2003
XX=    25.6759   YX=    -0.9013   ZX=     4.6770
XY=    -0.6524   YY=    27.4607   ZY=     5.2719
```

```
XZ=     2.5213   YZ=     0.6857   ZZ=    25.5565
Eigenvalues:    20.8850    27.4435    30.3646
  35  H    Isotropic =    30.2079   Anisotropy =     8.9325
XX=    26.9289   YX=     1.8953   ZX=     0.9723
XY=     2.5580   YY=    35.3994   ZY=    -0.3966
XZ=     0.2613   YZ=    -2.5641   ZZ=    28.2954
Eigenvalues:    25.9600    28.5008    36.1629
  36  H    Isotropic =    30.2085   Anisotropy =     6.7963
XX=    27.7716   YX=    -0.2423   ZX=    -3.8198
XY=    -1.2890   YY=    29.8238   ZY=    -1.4942
XZ=    -2.9819   YZ=    -0.2311   ZZ=    33.0299
Eigenvalues:    25.8163    30.0698    34.7393
  37  H    Isotropic =    30.0243   Anisotropy =     7.2943
XX=    31.2583   YX=    -0.5302   ZX=     2.1253
XY=    -1.7650   YY=    30.3992   ZY=    -4.1824
XZ=     2.9505   YZ=    -3.0159   ZZ=    28.4155
Eigenvalues:    25.3342    29.8516    34.8872
  38  H    Isotropic =    24.4538   Anisotropy =    23.5799
XX=    35.3070   YX=     4.5960   ZX=    -8.6773
XY=     8.6305   YY=    15.3261   ZY=     2.2299
XZ=    -6.9453   YZ=     1.3532   ZZ=    22.7283
Eigenvalues:    11.6273    21.5604    40.1737
  39  H    Isotropic =    28.0936   Anisotropy =    14.7122
XX=    32.0002   YX=     0.1104   ZX=     4.9383
XY=     0.9262   YY=    20.7723   ZY=     3.4384
XZ=     6.6191   YZ=     2.6338   ZZ=    31.5084
Eigenvalues:    19.8742    26.5049    37.9018
  40  H    Isotropic =    29.6588   Anisotropy =     8.1262
XX=    30.9665   YX=    -2.6970   ZX=    -2.5139
XY=    -2.2272   YY=    28.0770   ZY=     4.3426
XZ=    -0.4696   YZ=     3.9541   ZZ=    29.9329
Eigenvalues:    24.5777    29.3223    35.0762
  41  H    Isotropic =    29.3892   Anisotropy =     8.7618
XX=    31.8115   YX=     2.9412   ZX=    -2.0822
XY=     4.1740   YY=    29.1048   ZY=    -1.8705
XZ=    -2.3131   YZ=    -1.5344   ZZ=    27.2513
Eigenvalues:    26.2349    26.7024    35.2304
  42  H    Isotropic =    29.8578   Anisotropy =     8.1303
XX=    33.0304   YX=    -2.2537   ZX=     3.4447
XY=    -2.9438   YY=    25.6057   ZY=    -0.9551
XZ=     1.2900   YZ=    -0.5890   ZZ=    30.9373
Eigenvalues:    24.7864    29.5091    35.2780
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 50.80 | 68.94 | 83.03 | 98.82 | 123.87 | 154.61 |
| intensities | 0.11 | 0.17 | 0.71 | 0.40 | 0.37 | 1.21 |
| reduc. mass | 1.45 | 1.53 | 0.86 | 1.06 | 1.00 | 1.12 |
| force const | 0.00 | 0.00 | 0.00 | 0.01 | 0.01 | 0.02 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 179.71 | 206.63 | 241.36 | 246.64 | 262.42 | 263.77 |
| intensities | 1.80 | 0.95 | 1.34 | 1.29 | 4.32 | 0.82 |
| reduc. mass | 0.84 | 0.90 | 0.61 | 0.62 | 0.53 | 0.47 |
| force const | 0.02 | 0.02 | 0.02 | 0.02 | 0.02 | 0.02 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 277.75 | 294.30 | 302.58 | 318.90 | 322.07 | 365.71 |
| intensities | 1.22 | 0.21 | 0.89 | 0.60 | 0.70 | 10.14 |
| reduc. mass | 0.89 | 0.67 | 0.27 | 1.70 | 0.27 | 4.03 |
| force const | 0.04 | 0.03 | 0.01 | 0.10 | 0.02 | 0.32 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 372.48 | 406.64 | 438.63 | 447.47 | 485.61 | 515.90 |
| intensities | 0.08 | 1.25 | 2.65 | 11.40 | 3.70 | 15.27 |
| reduc. mass | 0.25 | 0.57 | 0.61 | 1.23 | 0.79 | 0.67 |
| force const | 0.02 | 0.06 | 0.07 | 0.15 | 0.11 | 0.10 |
| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 521.20 | 527.90 | 533.31 | 562.91 | 587.49 | 602.88 |
| intensities | 7.12 | 16.71 | 5.34 | 8.40 | 1.94 | 18.46 |
| reduc. mass | 2.72 | 0.68 | 0.79 | 0.60 | 1.12 | 0.49 |
| force const | 0.44 | 0.11 | 0.13 | 0.11 | 0.23 | 0.10 |

| | | | | | | |
|---|---|---|---|---|---|---|
| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
| frequencies | 636.14 | 674.83 | 712.43 | 719.77 | 730.68 | 742.47 |
| intensities | 9.67 | 19.87 | 6.84 | 29.59 | 33.34 | 1.90 |
| reduc. mass | 0.73 | 2.08 | 1.03 | 0.43 | 0.34 | 0.27 |
| force const | 0.17 | 0.56 | 0.31 | 0.13 | 0.11 | 0.09 |

| | | | | | | |
|---|---|---|---|---|---|---|
| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
| frequencies | 757.26 | 788.75 | 826.57 | 836.25 | 886.77 | 906.22 |
| intensities | 12.28 | 2.24 | 1.19 | 4.81 | 13.61 | 2.27 |
| reduc. mass | 1.36 | 1.08 | 2.35 | 0.59 | 0.71 | 0.72 |
| force const | 0.46 | 0.39 | 0.95 | 0.24 | 0.33 | 0.35 |

| | | | | | | |
|---|---|---|---|---|---|---|
| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
| frequencies | 928.49 | 943.18 | 956.68 | 991.70 | 1005.04 | 1016.91 |
| intensities | 0.05 | 0.76 | 19.71 | 1.33 | 4.12 | 34.32 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.73 | 1.63 | 0.70 | 0.26 | 0.28 | 0.37 |
| force const | 0.37 | 0.86 | 0.38 | 0.15 | 0.17 | 0.22 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1028.79 | 1041.48 | 1046.07 | 1056.29 | 1080.31 | 1097.99 |
| intensities | 35.43 | 7.23 | 4.50 | 4.76 | 18.93 | 29.09 |
| reduc. mass | 0.45 | 0.57 | 0.27 | 0.41 | 0.47 | 0.56 |
| force const | 0.28 | 0.37 | 0.17 | 0.27 | 0.33 | 0.40 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1114.89 | 1121.44 | 1143.86 | 1155.08 | 1177.17 | 1211.30 |
| intensities | 19.12 | 18.04 | 4.87 | 41.52 | 6.22 | 20.03 |
| reduc. mass | 0.36 | 0.44 | 0.37 | 0.61 | 0.39 | 0.67 |
| force const | 0.26 | 0.33 | 0.29 | 0.48 | 0.32 | 0.58 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1250.37 | 1258.22 | 1263.68 | 1265.80 | 1277.94 | 1317.95 |
| intensities | 62.42 | 90.35 | 38.06 | 1.96 | 14.58 | 9.08 |
| reduc. mass | 0.94 | 0.51 | 0.83 | 0.34 | 0.65 | 0.63 |
| force const | 0.87 | 0.48 | 0.78 | 0.32 | 0.62 | 0.64 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1351.28 | 1375.77 | 1413.69 | 1430.63 | 1463.11 | 1499.40 |
| intensities | 32.43 | 31.46 | 431.12 | 8.62 | 26.67 | 2.19 |
| reduc. mass | 1.00 | 0.45 | 1.05 | 0.49 | 0.79 | 0.67 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 1.08 | 0.50 | 1.23 | 0.59 | 1.00 | 0.88 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1503.26 | 1506.94 | 1522.96 | 1529.26 | 1547.40 | 1559.58 |
| intensities | 13.00 | 13.54 | 32.64 | 2.91 | 17.87 | 21.13 |
| reduc. mass | 0.52 | 1.78 | 1.15 | 2.48 | 0.64 | 0.81 |
| force const | 0.69 | 2.38 | 1.58 | 3.41 | 0.90 | 1.16 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1572.73 | 1596.73 | 1606.72 | 1638.55 | 1645.13 | 1648.07 |
| intensities | 61.97 | 11.95 | 4.15 | 4.27 | 55.94 | 55.17 |
| reduc. mass | 1.05 | 0.72 | 0.58 | 0.81 | 0.40 | 0.44 |
| force const | 1.53 | 1.09 | 0.88 | 1.29 | 0.63 | 0.71 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1657.14 | 1658.12 | 1660.04 | 1661.79 | 1667.80 | 1670.37 |
| intensities | 13.13 | 14.90 | 25.41 | 44.64 | 22.40 | 52.76 |
| reduc. mass | 0.16 | 0.20 | 0.27 | 0.33 | 0.42 | 0.66 |
| force const | 0.26 | 0.32 | 0.44 | 0.54 | 0.69 | 1.09 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1676.95 | 1681.93 | 1683.03 | 1684.61 | 1791.22 | 1822.10 |
| intensities | 21.42 | 9.05 | 22.12 | 6.00 | 761.86 | 131.10 |
| reduc. mass | 0.55 | 0.38 | 0.30 | 0.32 | 1.34 | 1.06 |
| force const | 0.91 | 0.63 | 0.49 | 0.53 | 2.54 | 2.07 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1835.82 | 1896.20 | 3020.37 | 3025.21 | 3027.27 | 3055.79 |
| intensities | 82.39 | 15.94 | 225.24 | 528.35 | 880.66 | 414.72 |
| reduc. mass | 0.82 | 0.87 | 0.24 | 0.25 | 0.30 | 0.47 |
| force const | 1.64 | 1.85 | 1.28 | 1.35 | 1.61 | 2.59 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3057.14 | 3086.29 | 3094.84 | 3107.44 | 3122.41 | 3124.06 |
| intensities | 642.72 | 333.03 | 372.38 | 76.20 | 32.05 | 447.15 |
| reduc. mass | 0.45 | 0.47 | 0.35 | 0.45 | 0.43 | 0.43 |
| force const | 2.50 | 2.65 | 1.97 | 2.55 | 2.47 | 2.46 |

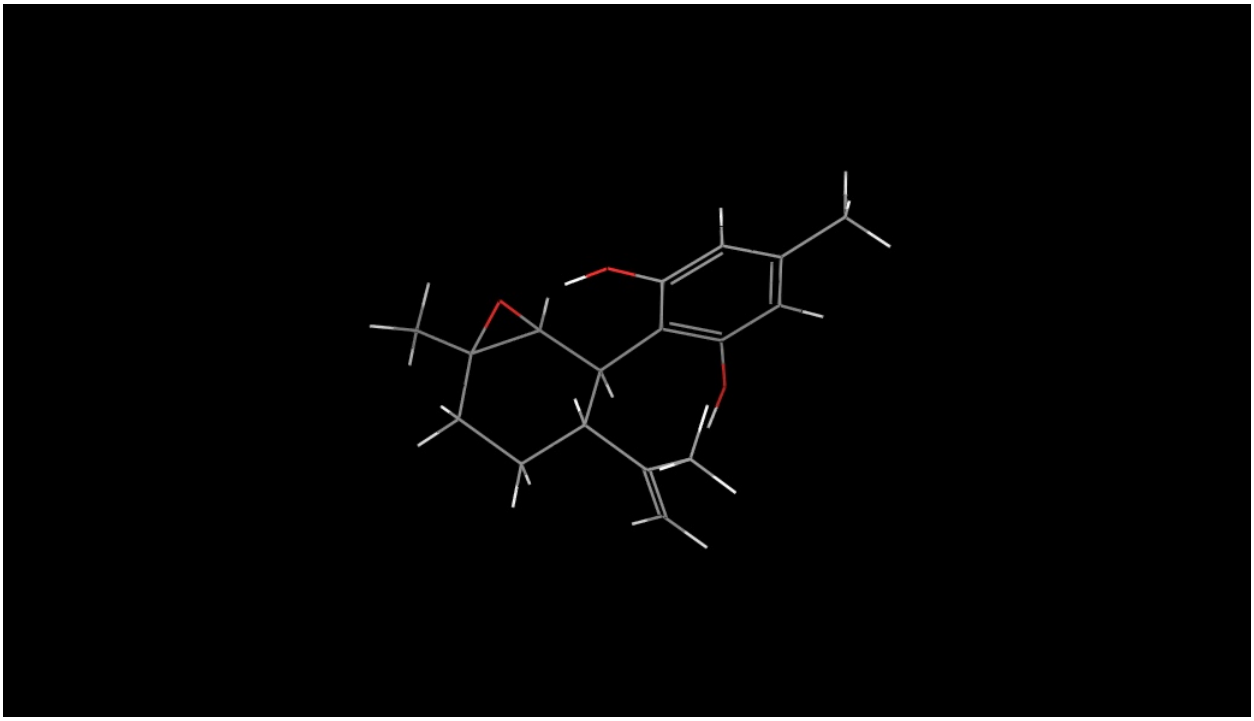
| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3124.59 | 3127.58 | 3134.30 | 3135.94 | 3138.14 | 3143.44 |
| intensities | 535.42 | 235.13 | 236.03 | 494.09 | 349.49 | 364.78 |
| reduc. mass | 0.24 | 0.34 | 0.75 | 0.47 | 0.52 | 0.57 |
| force const | 1.36 | 1.95 | 4.36 | 2.72 | 3.00 | 3.30 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3147.23 | 3149.92 | 3154.36 | 3206.36 | 3820.23 | 3856.98 |
| intensities | 307.86 | 454.56 | 440.07 | 309.81 | 524.00 | 23.16 |
| reduc. mass | 0.45 | 0.56 | 0.81 | 0.56 | 0.90 | 0.90 |
| force const | 2.64 | 3.26 | 4.77 | 3.39 | 7.74 | 7.92 |

Number of imaginary frequencies: 0

Conformation 4

Boltzmann Population = 3.6% (relative energy = 1.71 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot (SCFE + ZPE + U): -885.955157 hartrees

Total enthalpy, Htot (Utot + pV): -885.954213 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.016426 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.366100 | -2.532000 | 0.122700 |
| 2 | 6 | 0 | -0.281800 | -3.474600 | 0.646200 |
| 3 | 6 | 0 | -0.374100 | -3.665400 | 2.162500 |
| 4 | 6 | 0 | -0.109500 | -2.319500 | 2.880700 |

| | | | | | |
|---|---|---|---|---|---|
| 5 | 6 | 0 | -0.902800 | -1.172800 | 2.286400 |
| 6 | 6 | 0 | -1.488000 | -1.249700 | 0.932500 |
| 7 | 6 | 0 | -1.734800 | 0.017800 | 0.155100 |
| 8 | 6 | 0 | -0.242700 | -2.453500 | 4.388000 |
| 9 | 6 | 0 | -1.473800 | -2.680200 | 5.031000 |
| 10 | 6 | 0 | -1.533900 | -2.865700 | 6.413300 |
| 11 | 6 | 0 | -0.382400 | -2.838600 | 7.192000 |
| 12 | 6 | 0 | 0.848700 | -2.652600 | 6.565800 |
| 13 | 6 | 0 | 0.912700 | -2.484600 | 5.188000 |
| 14 | 6 | 0 | 0.591700 | -4.716600 | 2.694800 |
| 15 | 6 | 0 | 1.879200 | -4.736400 | 2.332000 |
| 16 | 6 | 0 | 0.020400 | -5.720200 | 3.657600 |
| 17 | 8 | 0 | -2.655500 | -2.792100 | 4.375300 |
| 18 | 8 | 0 | 2.163300 | -2.350700 | 4.634000 |
| 19 | 6 | 0 | -0.463700 | -3.008100 | 8.687200 |
| 20 | 8 | 0 | -2.310000 | -1.364100 | 2.104400 |
| 21 | 1 | 0 | -1.161800 | -2.275700 | -0.921700 |
| 22 | 1 | 0 | -2.345000 | -3.025400 | 0.142000 |
| 23 | 1 | 0 | 0.702800 | -3.056700 | 0.401100 |
| 24 | 1 | 0 | -0.347100 | -4.443000 | 0.140800 |
| 25 | 1 | 0 | -1.393300 | -3.988000 | 2.414700 |
| 26 | 1 | 0 | 0.934200 | -2.051100 | 2.675000 |
| 27 | 1 | 0 | -0.647500 | -0.189500 | 2.682700 |
| 28 | 1 | 0 | -1.891200 | 0.857800 | 0.834500 |
| 29 | 1 | 0 | -0.882900 | 0.238100 | -0.494300 |
| 30 | 1 | 0 | -2.623800 | -0.093300 | -0.473000 |
| 31 | 1 | 0 | -2.510100 | -3.035100 | 6.856200 |
| 32 | 1 | 0 | 1.778200 | -2.667100 | 7.125000 |
| 33 | 1 | 0 | 2.560300 | -5.487700 | 2.719800 |
| 34 | 1 | 0 | 2.289800 | -4.030000 | 1.614400 |
| 35 | 1 | 0 | 0.783300 | -6.413800 | 4.017400 |
| 36 | 1 | 0 | -0.432600 | -5.213900 | 4.517100 |
| 37 | 1 | 0 | -0.774200 | -6.296900 | 3.170500 |
| 38 | 1 | 0 | -2.617500 | -2.422900 | 3.477800 |
| 39 | 1 | 0 | 2.240500 | -2.997700 | 3.916500 |
| 40 | 1 | 0 | -1.320400 | -3.625000 | 8.968300 |
| 41 | 1 | 0 | 0.442400 | -3.475200 | 9.080500 |
| 42 | 1 | 0 | -0.577000 | -2.037800 | 9.181300 |

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```
SCF GIAO Magnetic shielding tensor (ppm):
      1  C    Isotropic =   154.8659   Anisotropy =    24.1925
   XX=   149.3084   YX=    -3.6678   ZX=     2.8445
   XY=    -3.1348   YY=   164.8935   ZY=   -10.5815
   XZ=    -4.3736   YZ=   -11.0619   ZZ=   150.3959
   Eigenvalues:   143.6587   149.9449   170.9943
      2  C    Isotropic =   155.6046   Anisotropy =    15.8312
   XX=   165.7607   YX=     1.6299   ZX=     1.9208
   XY=     0.2931   YY=   157.8694   ZY=     6.0336
   XZ=     2.5720   YZ=    -1.2108   ZZ=   143.1837
   Eigenvalues:   142.6126   158.0425   166.1587
```

```
   3  C    Isotropic =   146.6448   Anisotropy =    24.9574
XX=   156.9102   YX=    12.0256   ZX=     2.5345
XY=     7.0164   YY=   148.7115   ZY=     4.3028
XZ=     1.5984   YZ=    -4.2090   ZZ=   134.3125
Eigenvalues:   134.0635   142.5877   163.2830
   4  C    Isotropic =   140.5221   Anisotropy =    31.1489
XX=   123.6916   YX=    -0.6765   ZX=     5.0155
XY=    -2.7412   YY=   156.1344   ZY=    -5.7632
XZ=     1.7331   YZ=   -13.6973   ZZ=   141.7403
Eigenvalues:   123.0813   137.1970   161.2880
   5  C    Isotropic =   121.4171   Anisotropy =    53.8615
XX=    95.2576   YX=    11.5804   ZX=   -19.3808
XY=    13.0643   YY=   142.6593   ZY=    -8.7653
XZ=   -22.1859   YZ=   -17.2541   ZZ=   126.3345
Eigenvalues:    84.3352   122.5914   157.3248
   6  C    Isotropic =   125.7156   Anisotropy =    56.2861
XX=    83.9812   YX=     4.8692   ZX=   -25.0428
XY=     1.0232   YY=   155.7348   ZY=   -10.6593
XZ=   -29.0974   YZ=    -9.4633   ZZ=   137.4308
Eigenvalues:    72.6499   141.2572   163.2397
   7  C    Isotropic =   162.2211   Anisotropy =    43.1964
XX=   168.6574   YX=     7.7515   ZX=   -17.2738
XY=     7.7830   YY=   168.3135   ZY=   -21.0071
XZ=   -12.3788   YZ=   -18.8984   ZZ=   149.6923
Eigenvalues:   134.6298   161.0148   191.0187
   8  C    Isotropic =    70.2612   Anisotropy =   125.9227
XX=    19.3345   YX=    15.3222   ZX=     3.3957
XY=    16.0391   YY=   109.2074   ZY=   -55.3858
XZ=    -2.1837   YZ=   -56.2433   ZZ=    82.2416
Eigenvalues:    14.0413    42.5326   154.2096
   9  C    Isotropic =    24.1354   Anisotropy =   139.5706
XX=   -16.2174   YX=   -14.7170   ZX=   -38.7239
XY=    -8.2818   YY=    69.8015   ZY=   -66.7017
XZ=   -39.8135   YZ=   -66.9804   ZZ=    18.8222
Eigenvalues:   -61.3710    16.5948   117.1825
  10  C    Isotropic =    70.3669   Anisotropy =   120.7595
XX=    66.3121   YX=    17.1239   ZX=    11.1766
XY=    27.8741   YY=    90.8732   ZY=   -74.1247
XZ=     8.6841   YZ=   -75.0216   ZZ=    53.9153
Eigenvalues:   -10.6149    70.8423   150.8732
  11  C    Isotropic =    41.7648   Anisotropy =   196.7852
XX=   -53.0209   YX=    25.6705   ZX=     0.0948
XY=    16.7351   YY=   107.3222   ZY=   -81.2168
XZ=     4.8360   YZ=   -80.3356   ZZ=    70.9931
Eigenvalues:   -57.6014     9.9409   172.9549
  12  C    Isotropic =    70.5916   Anisotropy =   121.8384
XX=    38.6585   YX=   -16.1109   ZX=   -36.6279
XY=   -24.3427   YY=    95.1097   ZY=   -70.3346
XZ=   -37.8926   YZ=   -57.3077   ZZ=    78.0067
Eigenvalues:   -11.9772    71.9349   151.8173
  13  C    Isotropic =    27.2563   Anisotropy =   132.9406
XX=    25.9972   YX=    25.2220   ZX=    11.3439
```

```
XY=    28.3586   YY=    32.3332   ZY=   -84.9780
XZ=     4.2761   YZ=   -86.2231   ZZ=    23.4386
Eigenvalues:   -64.3442    30.2298   115.8834
  14  C    Isotropic =    15.3731   Anisotropy =   213.5424
XX=     5.2717   YX=   -80.2034   ZX=   106.9063
XY=   -86.6262   YY=    16.8147   ZY=   -14.9765
XZ=   102.7873   YZ=   -23.5212   ZZ=    24.0329
Eigenvalues:  -112.4719     0.8565   157.7348
  15  C    Isotropic =    76.9695   Anisotropy =   126.2480
XX=    54.1133   YX=   -68.0167   ZX=    64.3466
XY=   -70.2044   YY=    76.6656   ZY=     9.9584
XZ=    65.9688   YZ=    15.8848   ZZ=   100.1296
Eigenvalues:   -31.4860   101.2597   161.1348
  16  C    Isotropic =   158.5232   Anisotropy =    42.3901
XX=   163.8864   YX=    11.4730   ZX=   -21.1560
XY=     6.1573   YY=   149.6118   ZY=    -4.9128
XZ=   -21.0564   YZ=    -5.4849   ZZ=   162.0714
Eigenvalues:   140.9849   147.8015   186.7833
  17  O    Isotropic =   204.2604   Anisotropy =    79.0944
XX=   167.2890   YX=    11.3180   ZX=    14.5862
XY=    34.0226   YY=   217.0114   ZY=   -50.9277
XZ=    15.5936   YZ=   -16.3478   ZZ=   228.4808
Eigenvalues:   148.8115   206.9797   256.9900
  18  O    Isotropic =   226.3608   Anisotropy =    76.1577
XX=   178.1250   YX=     1.1161   ZX=   -25.2368
XY=   -12.2243   YY=   244.0279   ZY=   -43.0803
XZ=    -3.7286   YZ=    -7.2497   ZZ=   256.9296
Eigenvalues:   174.0087   227.9412   277.1326
  19  C    Isotropic =   164.1945   Anisotropy =    40.6947
XX=   189.4245   YX=    -3.7855   ZX=    -6.1934
XY=   -10.7446   YY=   149.9353   ZY=     8.3419
XZ=    -0.6852   YZ=     7.0029   ZZ=   153.2237
Eigenvalues:   143.4480   157.8113   191.3243
  20  O    Isotropic =   259.9118   Anisotropy =   135.4883
XX=   331.2055   YX=     9.6387   ZX=     1.6000
XY=    33.4741   YY=   249.3405   ZY=  -124.0005
XZ=     5.5163   YZ=   -98.5492   ZZ=   199.1894
Eigenvalues:   109.0074   320.4906   350.2374
  21  H    Isotropic =    29.8980   Anisotropy =     8.6163
XX=    35.4375   YX=    -0.3844   ZX=    -1.3822
XY=    -1.3357   YY=    29.3117   ZY=    -1.1792
XZ=    -0.8254   YZ=    -0.9186   ZZ=    24.9447
Eigenvalues:    24.5573    29.4945    35.6422
  22  H    Isotropic =    29.9184   Anisotropy =     7.8988
XX=    28.4162   YX=     1.2488   ZX=     3.3058
XY=    -0.1983   YY=    28.1801   ZY=    -0.1252
XZ=     4.0254   YZ=     0.6143   ZZ=    33.1588
Eigenvalues:    26.3558    28.2150    35.1843
  23  H    Isotropic =    30.1675   Anisotropy =     7.3186
XX=    30.3272   YX=     0.0029   ZX=    -1.8075
XY=    -0.3776   YY=    31.8433   ZY=     5.0324
XZ=    -1.0181   YZ=     3.8236   ZZ=    28.3320
```

```
Eigenvalues:    25.1038    30.3521    35.0466
  24  H    Isotropic =    30.2917   Anisotropy =     9.3730
XX=    30.5150   YX=    -1.5826   ZX=     2.1740
XY=    -2.2585   YY=    32.5342   ZY=    -4.2696
XZ=     3.3143   YZ=    -4.0479   ZZ=    27.8259
Eigenvalues:    24.9744    29.3603    36.5404
  25  H    Isotropic =    29.3150   Anisotropy =     3.6737
XX=    29.0890   YX=     1.1271   ZX=    -2.0990
XY=    -1.4763   YY=    28.5806   ZY=     0.1096
XZ=    -1.8886   YZ=    -0.1843   ZZ=    30.2754
Eigenvalues:    27.5757    28.6051    31.7641
  26  H    Isotropic =    28.2747   Anisotropy =     9.0231
XX=    29.5127   YX=     1.9485   ZX=     3.1546
XY=     3.5518   YY=    26.9576   ZY=     3.5601
XZ=     2.4242   YZ=     3.1816   ZZ=    28.3536
Eigenvalues:    24.1694    26.3645    34.2901
  27  H    Isotropic =    28.8175   Anisotropy =    10.0657
XX=    26.0799   YX=     3.5787   ZX=     0.0592
XY=     2.0061   YY=    28.3655   ZY=    -5.7728
XZ=     1.9075   YZ=    -4.1174   ZZ=    32.0070
Eigenvalues:    22.5671    28.3573    35.5280
  28  H    Isotropic =    31.1452   Anisotropy =    10.6167
XX=    29.5719   YX=     1.1573   ZX=    -0.8871
XY=     1.1353   YY=    34.4610   ZY=    -5.6102
XZ=    -0.7952   YZ=    -5.4001   ZZ=    29.4027
Eigenvalues:    25.8712    29.3414    38.2230
  29  H    Isotropic =    30.3200   Anisotropy =    10.1531
XX=    31.8814   YX=    -0.9603   ZX=    -5.4203
XY=     0.8957   YY=    27.7108   ZY=     0.2437
XZ=    -5.4499   YZ=     1.0321   ZZ=    31.3678
Eigenvalues:    26.0648    27.8065    37.0888
  30  H    Isotropic =    30.1155   Anisotropy =     9.5472
XX=    33.2925   YX=     3.9171   ZX=     2.2593
XY=     5.1255   YY=    29.2883   ZY=     0.7287
XZ=     0.6714   YZ=     0.1217   ZZ=    27.7657
Eigenvalues:    26.2006    27.6656    36.4803
  31  H    Isotropic =    25.0369   Anisotropy =     7.4967
XX=    29.7889   YX=    -0.2219   ZX=     1.3331
XY=    -0.4869   YY=    22.3415   ZY=     0.9456
XZ=     1.2893   YZ=     1.5219   ZZ=    22.9803
Eigenvalues:    21.2451    23.8309    30.0347
  32  H    Isotropic =    25.1057   Anisotropy =     6.9819
XX=    28.1384   YX=    -2.4979   ZX=    -1.3563
XY=    -2.0031   YY=    23.4447   ZY=     2.1570
XZ=    -1.3665   YZ=     1.9628   ZZ=    23.7342
Eigenvalues:    21.4253    24.1316    29.7603
  33  H    Isotropic =    26.7496   Anisotropy =     5.8853
XX=    24.4336   YX=    -1.5764   ZX=    -0.3547
XY=    -0.1945   YY=    29.7750   ZY=     1.1141
XZ=     1.5367   YZ=     2.8143   ZZ=    26.0403
Eigenvalues:    23.8102    25.7656    30.6731
  34  H    Isotropic =    26.6143   Anisotropy =     8.2430
```

```
XX=    24.7620   YX=     0.6457   ZX=     2.0730
XY=    -2.3703   YY=    30.1489   ZY=     5.7145
XZ=     0.6046   YZ=     1.7813   ZZ=    24.9321
Eigenvalues:    22.0472    25.6861    32.1097
  35  H    Isotropic =    30.4284   Anisotropy =     8.5571
XX=    29.9899   YX=     4.6639   ZX=    -1.3459
XY=     2.5508   YY=    32.9053   ZY=    -0.6892
XZ=    -2.2525   YZ=    -2.8571   ZZ=    28.3899
Eigenvalues:    27.0992    28.0528    36.1331
  36  H    Isotropic =    30.7198   Anisotropy =     8.7609
XX=    29.9618   YX=    -2.9160   ZX=    -2.5680
XY=    -3.9166   YY=    33.4465   ZY=    -4.4812
XZ=    -0.2910   YZ=    -3.3516   ZZ=    28.7512
Eigenvalues:    24.7319    30.8672    36.5604
  37  H    Isotropic =    30.2802   Anisotropy =     8.5427
XX=    27.5577   YX=     0.5490   ZX=     0.2439
XY=     0.2869   YY=    28.0991   ZY=    -3.1045
XZ=     1.1785   YZ=    -1.7600   ZZ=    35.1839
Eigenvalues:    26.8177    28.0476    35.9753
  38  H    Isotropic =    24.2995   Anisotropy =    25.6806
XX=    38.2309   YX=     0.4261   ZX=    -8.7329
XY=     3.5841   YY=    15.8524   ZY=     5.2146
XZ=    -8.2412   YZ=     4.1533   ZZ=    18.8151
Eigenvalues:    10.6484    20.8301    41.4199
  39  H    Isotropic =    27.7464   Anisotropy =    18.1932
XX=    26.4464   YX=    -5.9582   ZX=     7.0669
XY=    -9.2563   YY=    32.5233   ZY=    -0.6540
XZ=     7.2412   YZ=    -3.2214   ZZ=    24.2696
Eigenvalues:    17.1243    26.2398    39.8752
  40  H    Isotropic =    29.6983   Anisotropy =     7.7846
XX=    31.4949   YX=    -1.6603   ZX=    -3.3278
XY=    -0.0974   YY=    25.6138   ZY=     2.4204
XZ=    -1.6571   YZ=     2.5136   ZZ=    31.9861
Eigenvalues:    24.7702    29.4366    34.8880
  41  H    Isotropic =    29.6734   Anisotropy =     7.9348
XX=    33.5389   YX=     3.1176   ZX=     1.3354
XY=     1.9231   YY=    29.0743   ZY=     2.6784
XZ=    -0.4152   YZ=     2.6274   ZZ=    26.4070
Eigenvalues:    24.6622    29.3948    34.9633
  42  H    Isotropic =    29.3167   Anisotropy =     9.2168
XX=    30.3388   YX=    -3.5344   ZX=     1.6655
XY=    -4.6083   YY=    30.4109   ZY=    -1.8272
XZ=     2.5230   YZ=    -2.1745   ZZ=    27.2005
Eigenvalues:    26.1496    26.3393    35.4613
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 59.71 | 65.48 | 82.17 | 106.33 | 119.69 | 148.21 |
| intensities | 0.16 | 0.41 | 1.30 | 1.20 | 1.44 | 0.96 |
| reduc. mass | 0.98 | 1.31 | 1.46 | 2.10 | 1.05 | 0.95 |
| force const | 0.00 | 0.00 | 0.01 | 0.01 | 0.01 | 0.01 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 181.41 | 194.01 | 229.80 | 237.83 | 242.70 | 255.15 |
| intensities | 1.64 | 0.97 | 0.29 | 3.43 | 1.01 | 9.60 |
| reduc. mass | 0.52 | 0.93 | 0.52 | 0.55 | 0.56 | 0.68 |
| force const | 0.01 | 0.02 | 0.02 | 0.02 | 0.02 | 0.03 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 278.77 | 298.10 | 300.03 | 318.29 | 327.27 | 368.30 |
| intensities | 0.26 | 1.03 | 2.31 | 5.86 | 0.27 | 0.74 |
| reduc. mass | 0.95 | 0.49 | 0.52 | 1.43 | 0.27 | 0.25 |
| force const | 0.04 | 0.03 | 0.03 | 0.09 | 0.02 | 0.02 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 373.33 | 396.91 | 441.79 | 458.43 | 486.58 | 506.25 |
| intensities | 1.22 | 2.03 | 6.37 | 4.24 | 9.28 | 2.89 |
| reduc. mass | 4.07 | 0.37 | 0.94 | 0.98 | 0.36 | 0.75 |
| force const | 0.33 | 0.03 | 0.11 | 0.12 | 0.05 | 0.11 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 521.72 | 524.47 | 526.94 | 535.69 | 551.18 | 584.96 |
| intensities | 4.77 | 21.40 | 15.20 | 5.67 | 2.55 | 8.73 |
| reduc. mass | 0.58 | 0.46 | 0.84 | 1.05 | 0.65 | 1.56 |
| force const | 0.09 | 0.07 | 0.14 | 0.18 | 0.12 | 0.31 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 625.53 | 694.37 | 712.58 | 714.48 | 728.05 | 745.38 |
| intensities | 7.24 | 1.75 | 10.51 | 3.87 | 17.26 | 15.00 |
| reduc. mass | 0.82 | 1.30 | 0.24 | 0.55 | 0.33 | 0.44 |
| force const | 0.19 | 0.37 | 0.07 | 0.17 | 0.10 | 0.14 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 759.13 | 791.11 | 805.28 | 833.57 | 878.66 | 904.97 |
| intensities | 5.37 | 4.68 | 12.83 | 5.33 | 7.54 | 3.05 |
| reduc. mass | 1.79 | 0.69 | 2.00 | 0.72 | 0.76 | 0.58 |
| force const | 0.61 | 0.25 | 0.76 | 0.30 | 0.35 | 0.28 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 935.76 | 943.69 | 948.38 | 994.44 | 1002.99 | 1012.16 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 0.07 | 3.17 | 14.36 | 9.63 | 8.22 | 23.95 |
| reduc. mass | 0.72 | 1.39 | 0.69 | 0.32 | 0.31 | 0.29 |
| force const | 0.37 | 0.73 | 0.36 | 0.19 | 0.18 | 0.17 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1030.52 | 1034.57 | 1044.47 | 1052.62 | 1057.18 | 1096.89 |
| intensities | 16.58 | 15.84 | 10.01 | 0.51 | 9.38 | 44.25 |
| reduc. mass | 0.51 | 0.58 | 0.40 | 0.29 | 0.55 | 0.68 |
| force const | 0.32 | 0.37 | 0.26 | 0.19 | 0.36 | 0.48 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1112.96 | 1122.18 | 1139.74 | 1147.06 | 1186.83 | 1209.34 |
| intensities | 5.13 | 7.95 | 26.25 | 5.15 | 6.35 | 17.73 |
| reduc. mass | 0.48 | 0.59 | 0.29 | 0.36 | 0.34 | 0.35 |
| force const | 0.35 | 0.44 | 0.22 | 0.28 | 0.29 | 0.30 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1251.35 | 1253.77 | 1260.61 | 1269.56 | 1285.49 | 1305.21 |
| intensities | 56.78 | 103.33 | 23.05 | 12.14 | 65.60 | 18.57 |
| reduc. mass | 0.83 | 0.47 | 0.77 | 0.24 | 0.63 | 0.57 |
| force const | 0.77 | 0.43 | 0.72 | 0.23 | 0.61 | 0.57 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1348.24 | 1379.12 | 1391.19 | 1432.08 | 1450.56 | 1467.97 |
| intensities | 32.77 | 59.88 | 326.83 | 25.72 | 14.21 | 2.21 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.94 | 0.41 | 1.31 | 0.58 | 0.79 | 0.74 |
| force const | 1.01 | 0.46 | 1.50 | 0.70 | 0.98 | 0.94 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1505.08 | 1512.23 | 1515.64 | 1524.47 | 1530.24 | 1560.42 |
| intensities | 2.06 | 59.32 | 21.12 | 22.52 | 14.32 | 14.72 |
| reduc. mass | 0.96 | 0.70 | 0.80 | 2.69 | 0.90 | 0.89 |
| force const | 1.28 | 0.94 | 1.08 | 3.68 | 1.24 | 1.27 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1572.25 | 1591.74 | 1611.12 | 1637.51 | 1642.91 | 1645.21 |
| intensities | 54.47 | 14.58 | 7.31 | 14.01 | 46.23 | 40.23 |
| reduc. mass | 1.26 | 0.75 | 0.94 | 0.61 | 0.27 | 0.34 |
| force const | 1.83 | 1.12 | 1.43 | 0.97 | 0.42 | 0.54 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1658.76 | 1660.26 | 1661.54 | 1664.80 | 1666.74 | 1669.94 |
| intensities | 41.78 | 54.66 | 54.05 | 12.61 | 23.87 | 68.87 |
| reduc. mass | 0.14 | 0.25 | 0.28 | 0.17 | 0.25 | 0.32 |
| force const | 0.22 | 0.41 | 0.45 | 0.28 | 0.41 | 0.52 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1674.13 | 1682.28 | 1682.71 | 1684.36 | 1792.32 | 1823.19 |
| intensities | 301.52 | 16.47 | 14.65 | 0.83 | 694.77 | 123.04 |
| reduc. mass | 1.07 | 0.37 | 0.37 | 0.31 | 1.34 | 0.98 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 1.76 | 0.62 | 0.62 | 0.52 | 2.54 | 1.93 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1831.17 | 1887.44 | 3022.30 | 3025.95 | 3028.54 | 3058.64 |
| intensities | 106.50 | 18.87 | 299.31 | 505.88 | 753.30 | 271.68 |
| reduc. mass | 0.80 | 0.85 | 0.33 | 0.32 | 0.33 | 0.25 |
| force const | 1.57 | 1.79 | 1.76 | 1.75 | 1.78 | 1.40 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3060.33 | 3079.86 | 3089.92 | 3093.58 | 3123.60 | 3126.25 |
| intensities | 651.90 | 140.50 | 131.68 | 344.95 | 532.36 | 445.10 |
| reduc. mass | 0.25 | 0.66 | 0.55 | 0.39 | 0.75 | 0.27 |
| force const | 1.36 | 3.67 | 3.11 | 2.22 | 4.29 | 1.56 |

| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3126.98 | 3129.45 | 3136.04 | 3139.23 | 3145.91 | 3146.57 |
| intensities | 196.59 | 101.19 | 455.12 | 372.86 | 99.74 | 265.41 |
| reduc. mass | 0.19 | 0.23 | 0.44 | 0.51 | 0.40 | 0.33 |
| force const | 1.09 | 1.33 | 2.55 | 2.94 | 2.33 | 1.90 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3150.40 | 3152.52 | 3155.08 | 3196.48 | 3822.12 | 3841.65 |
| intensities | 364.43 | 522.67 | 333.50 | 312.34 | 67.63 | 631.15 |
| reduc. mass | 0.55 | 0.70 | 0.78 | 0.56 | 0.79 | 0.79 |
| force const | 3.19 | 4.11 | 4.57 | 3.35 | 6.83 | 6.88 |

Number of imaginary frequencies: 0

3. DFT calculation data for CBE (**7**). Energies, optimized geometries, NMR shielding values and IR frequencies from calculations performed at the mPW1PW91/6-311+G(2d,p)//M06-2X-D3/6-31G(d,p) level.

Conformation 1

Boltzmann Population = 10.0% (relative energy = 0.84 kcal/mol)

Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.982145 hartrees

Total enthalpy, Htot (Utot + pV): -885.981201 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.044495 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.053400 | -0.679900 | -2.574100 |
| 2 | 6 | 0 | -4.599000 | -0.352800 | -2.899800 |
| 3 | 6 | 0 | -3.871300 | -1.608000 | -3.395500 |
| 4 | 6 | 0 | -3.939800 | -2.766100 | -2.359700 |
| 5 | 6 | 0 | -5.345000 | -2.952500 | -1.747000 |
| 6 | 6 | 0 | -6.136600 | -1.688200 | -1.425100 |
| 7 | 6 | 0 | -7.580100 | -2.034000 | -1.079300 |
| 8 | 6 | 0 | -2.432200 | -1.337600 | -3.783100 |
| 9 | 6 | 0 | -3.821200 | -4.109600 | -3.053300 |
| 10 | 6 | 0 | -5.118800 | -4.584200 | -3.256500 |
| 11 | 6 | 0 | -2.758200 | -4.850100 | -3.554400 |
| 12 | 6 | 0 | -3.023500 | -6.050200 | -4.228100 |
| 13 | 6 | 0 | -4.326700 | -6.497900 | -4.423000 |
| 14 | 6 | 0 | -5.409000 | -5.751900 | -3.932900 |
| 15 | 8 | 0 | -1.456600 | -4.486300 | -3.405000 |
| 16 | 8 | 0 | -6.060100 | -3.761200 | -2.696200 |
| 17 | 8 | 0 | -5.460100 | -1.177500 | -0.277000 |
| 18 | 6 | 0 | -4.589000 | -7.797800 | -5.141600 |
| 19 | 6 | 0 | -1.596500 | -0.526900 | -2.824300 |
| 20 | 6 | 0 | -1.924800 | -1.816900 | -4.922700 |
| 21 | 1 | 0 | -6.557700 | -1.101300 | -3.452200 |
| 22 | 1 | 0 | -6.604700 | 0.226000 | -2.290000 |
| 23 | 1 | 0 | -4.539500 | 0.425800 | -3.668100 |
| 24 | 1 | 0 | -4.115000 | 0.034600 | -1.996700 |
| 25 | 1 | 0 | -4.399800 | -1.960800 | -4.290800 |
| 26 | 1 | 0 | -3.209700 | -2.606800 | -1.559300 |
| 27 | 1 | 0 | -5.248800 | -3.530200 | -0.816500 |
| 28 | 1 | 0 | -8.087000 | -2.487400 | -1.933100 |
| 29 | 1 | 0 | -8.122900 | -1.126200 | -0.792500 |
| 30 | 1 | 0 | -7.607100 | -2.734600 | -0.240400 |
| 31 | 1 | 0 | -2.179100 | -6.617400 | -4.605600 |
| 32 | 1 | 0 | -6.433900 | -6.082600 | -4.060100 |
| 33 | 1 | 0 | -1.418800 | -3.524600 | -3.310300 |
| 34 | 1 | 0 | -5.930700 | -0.386400 | 0.012200 |
| 35 | 1 | 0 | -3.691700 | -8.161000 | -5.646300 |
| 36 | 1 | 0 | -4.916300 | -8.570700 | -4.438900 |
| 37 | 1 | 0 | -5.379100 | -7.680200 | -5.888600 |
| 38 | 1 | 0 | -1.929300 | 0.516200 | -2.807700 |
| 39 | 1 | 0 | -1.682700 | -0.899300 | -1.797200 |
| 40 | 1 | 0 | -0.542600 | -0.541300 | -3.110200 |
| 41 | 1 | 0 | -0.887100 | -1.650700 | -5.198600 |
| 42 | 1 | 0 | -2.533900 | -2.396100 | -5.610800 |

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 149.2811 Anisotropy = 21.7909

XX= 143.9598 YX= -0.3783 ZX= 4.1016

XY= -5.3716 YY= 154.9419 ZY= 10.2980

XZ= -3.7946 YZ= 12.1621 ZZ= 148.9415

Eigenvalues: 139.4956 144.5393 163.8083

```
   2  C    Isotropic =   161.3098   Anisotropy =    15.7808
XX=   164.7477   YX=    -6.5929   ZX=     6.6928
XY=    -4.2933   YY=   163.2330   ZY=     0.2042
XZ=     8.5127   YZ=    -0.1942   ZZ=   155.9488
Eigenvalues:   150.8972   161.2020   171.8304
   3  C    Isotropic =   133.7456   Anisotropy =    14.3557
XX=   136.0301   YX=    -1.3723   ZX=     2.1666
XY=     6.7028   YY=   138.9162   ZY=    -6.4471
XZ=     0.5947   YZ=    -9.7176   ZZ=   126.2905
Eigenvalues:   121.9315   135.9892   143.3161
   4  C    Isotropic =   142.0035   Anisotropy =    19.3071
XX=   148.1547   YX=    -1.0212   ZX=     1.9211
XY=     0.2839   YY=   148.5372   ZY=     0.8722
XZ=     6.7819   YZ=    23.5762   ZZ=   129.3186
Eigenvalues:   122.7240   148.4116   154.8749
   5  C    Isotropic =    97.3419   Anisotropy =    58.0116
XX=   118.7459   YX=    10.1787   ZX=   -22.9858
XY=     1.9189   YY=    92.8559   ZY=   -20.4346
XZ=   -29.4971   YZ=   -11.9841   ZZ=    80.4238
Eigenvalues:    62.2439    93.7655   136.0162
   6  C    Isotropic =   115.6644   Anisotropy =    54.6768
XX=   116.3306   YX=    14.4211   ZX=   -29.8686
XY=    10.5508   YY=   110.3326   ZY=    -8.6302
XZ=   -26.1464   YZ=   -10.2556   ZZ=   120.3300
Eigenvalues:    89.8041   105.0735   152.1156
   7  C    Isotropic =   157.3878   Anisotropy =    45.4168
XX=   143.8699   YX=    -7.9502   ZX=     0.6007
XY=    -3.5024   YY=   186.7974   ZY=    -1.9287
XZ=    -1.1793   YZ=    -2.8468   ZZ=   141.4962
Eigenvalues:   141.1938   143.3039   187.6657
   8  C    Isotropic =    28.0506   Anisotropy =   193.1309
XX=    59.1680   YX=    -9.4959   ZX=    78.6473
XY=   -16.3816   YY=   -51.1938   ZY=    66.1586
XZ=    81.1313   YZ=    67.2240   ZZ=    76.1775
Eigenvalues:   -94.1739    21.5211   156.8045
   9  C    Isotropic =    66.5154   Anisotropy =   111.7026
XX=    20.3183   YX=     1.8441   ZX=     9.2526
XY=   -13.1667   YY=    58.6196   ZY=    37.1464
XZ=    21.6033   YZ=    42.0410   ZZ=   120.6081
Eigenvalues:    13.7943    44.7680   140.9838
  10  C    Isotropic =    20.7574   Anisotropy =   110.5817
XX=   -26.4435   YX=    36.8251   ZX=    -0.3993
XY=    46.4991   YY=     2.2071   ZY=    31.2053
XZ=    -9.7582   YZ=    21.4626   ZZ=    86.5085
Eigenvalues:   -58.8410    26.6346    94.4785
  11  C    Isotropic =    27.6875   Anisotropy =   134.1740
XX=    15.8754   YX=   -11.5488   ZX=    11.0705
XY=    -6.3950   YY=   -27.6147   ZY=    58.3961
XZ=     5.7080   YZ=    54.7187   ZZ=    94.8019
Eigenvalues:   -51.6757    17.6014   117.1369
  12  C    Isotropic =    72.2942   Anisotropy =   115.4800
XX=    24.0630   YX=    33.9802   ZX=    -4.4866
```

```
XY=    45.6171   YY=    53.7598   ZY=    34.7547
XZ=    -2.4895   YZ=    25.3930   ZZ=   139.0598
Eigenvalues:    -6.4364    74.0381   149.2809
  13  C    Isotropic =    41.6085   Anisotropy =   193.5731
XX=   -43.7328   YX=   -13.2555   ZX=    22.1433
XY=   -16.4870   YY=    26.7042   ZY=    61.5957
XZ=    28.9166   YZ=    63.3064   ZZ=   141.8540
Eigenvalues:   -55.4753     9.6435   170.6572
  14  C    Isotropic =    80.9834   Anisotropy =   123.0542
XX=    74.0598   YX=     5.2082   ZX=     6.4217
XY=   -10.5370   YY=    26.2964   ZY=    56.2853
XZ=     7.2384   YZ=    48.4189   ZZ=   142.5940
Eigenvalues:     5.8438    74.0868   163.0196
  15  O    Isotropic =   205.2124   Anisotropy =    79.7675
XX=   153.0105   YX=     2.1501   ZX=    -0.2541
XY=    13.8863   YY=   206.2646   ZY=    20.8606
XZ=    29.1334   YZ=   -19.8473   ZZ=   256.3622
Eigenvalues:   149.9297   207.3168   258.3908
  16  O    Isotropic =   188.5363   Anisotropy =   118.6810
XX=   216.4028   YX=   -68.6739   ZX=    32.8843
XY=   -50.9564   YY=   164.6923   ZY=    28.5952
XZ=    33.3436   YZ=   -41.8042   ZZ=   184.5139
Eigenvalues:   122.4510   175.5010   267.6570
  17  O    Isotropic =   248.6810   Anisotropy =    92.0953
XX=   309.2980   YX=    -0.4799   ZX=   -17.1269
XY=    -9.0954   YY=   206.9666   ZY=    -7.7844
XZ=     2.8530   YZ=   -13.3429   ZZ=   229.7785
Eigenvalues:   202.3567   233.6085   310.0779
  18  C    Isotropic =   163.9808   Anisotropy =    41.2779
XX=   187.4517   YX=     5.5354   ZX=    -9.1037
XY=    11.5733   YY=   157.3601   ZY=    -8.2053
XZ=    -5.5556   YZ=    -5.5105   ZZ=   147.1308
Eigenvalues:   143.4913   156.9518   191.4994
  19  C    Isotropic =   167.4021   Anisotropy =    27.0895
XX=   166.9322   YX=     5.6487   ZX=    -9.8875
XY=     8.8619   YY=   169.7591   ZY=   -11.5520
XZ=    -8.7747   YZ=    -9.1490   ZZ=   165.5151
Eigenvalues:   155.7462   160.9984   185.4618
  20  C    Isotropic =    66.0737   Anisotropy =   115.4512
XX=   104.5626   YX=   -22.1906   ZX=    34.2543
XY=   -17.9800   YY=    -5.1210   ZY=    56.9337
XZ=    39.9118   YZ=    50.2928   ZZ=    98.7795
Eigenvalues:   -35.8122    90.9921   143.0412
  21  H    Isotropic =    29.9188   Anisotropy =     6.1674
XX=    27.5783   YX=    -0.1998   ZX=    -1.1239
XY=     0.4814   YY=    29.0049   ZY=    -1.7327
XZ=     0.0877   YZ=    -2.2926   ZZ=    33.1731
Eigenvalues:    27.5282    28.1977    34.0303
  22  H    Isotropic =    30.4633   Anisotropy =     8.6660
XX=    33.0730   YX=    -2.7579   ZX=     3.9309
XY=    -2.3283   YY=    30.3679   ZY=    -0.2154
XZ=     4.0944   YZ=    -0.3535   ZZ=    27.9488
```

```
Eigenvalues:    25.5283    29.6209    36.2406
  23  H    Isotropic =    30.6196   Anisotropy =    10.0731
XX=    29.6435   YX=     1.1120   ZX=     4.6961
XY=     1.1506   YY=    31.1333   ZY=     3.5545
XZ=     5.5002   YZ=     3.2751   ZZ=    31.0821
Eigenvalues:    24.8485    29.6753    37.3350
  24  H    Isotropic =    29.6117   Anisotropy =     5.7936
XX=    30.5161   YX=     1.3113   ZX=    -2.5207
XY=     0.9617   YY=    32.1824   ZY=    -1.4351
XZ=    -2.0316   YZ=    -1.1868   ZZ=    26.1366
Eigenvalues:    25.0817    30.2794    33.4741
  25  H    Isotropic =    29.6369   Anisotropy =     2.4490
XX=    30.0070   YX=    -1.7039   ZX=    -1.4895
XY=     0.4263   YY=    28.7719   ZY=     0.3160
XZ=     0.3354   YZ=     1.8573   ZZ=    30.1317
Eigenvalues:    28.1222    29.5189    31.2695
  26  H    Isotropic =    28.5430   Anisotropy =     4.4112
XX=    26.9045   YX=     0.8349   ZX=     0.5511
XY=    -1.1101   YY=    29.3878   ZY=    -2.0045
XZ=    -0.9105   YZ=    -2.2378   ZZ=    29.3367
Eigenvalues:    26.7920    27.3532    31.4838
  27  H    Isotropic =    27.6482   Anisotropy =     4.9637
XX=    26.5728   YX=     0.7615   ZX=    -1.0084
XY=    -1.0024   YY=    27.5064   ZY=     1.0083
XZ=    -2.7447   YZ=     3.1043   ZZ=    28.8655
Eigenvalues:    25.0552    26.9322    30.9574
  28  H    Isotropic =    29.9439   Anisotropy =     8.4041
XX=    29.2772   YX=     0.4241   ZX=    -2.2855
XY=     0.9510   YY=    32.7298   ZY=    -4.4003
XZ=    -2.2195   YZ=    -3.8122   ZZ=    27.8246
Eigenvalues:    24.8593    29.4257    35.5466
  29  H    Isotropic =    30.9814   Anisotropy =     8.9109
XX=    33.0347   YX=    -3.3665   ZX=     1.4557
XY=    -4.6395   YY=    32.3086   ZY=    -0.7197
XZ=     1.3747   YZ=    -0.5257   ZZ=    27.6010
Eigenvalues:    27.2056    28.8166    36.9221
  30  H    Isotropic =    30.3502   Anisotropy =     9.1006
XX=    27.8259   YX=    -0.4282   ZX=     0.4428
XY=    -0.3511   YY=    33.7738   ZY=     4.9159
XZ=     0.2533   YZ=     3.6609   ZZ=    29.4508
Eigenvalues:    26.6044    28.0289    36.4173
  31  H    Isotropic =    25.2632   Anisotropy =     6.6998
XX=    27.3224   YX=     2.3032   ZX=    -1.1549
XY=     2.3414   YY=    26.0769   ZY=    -2.0295
XZ=    -0.9081   YZ=    -2.2234   ZZ=    22.3903
Eigenvalues:    21.4193    24.6405    29.7297
  32  H    Isotropic =    25.3252   Anisotropy =     7.5743
XX=    30.2810   YX=     0.0291   ZX=    -0.7840
XY=     0.5874   YY=    24.0356   ZY=    -1.1448
XZ=    -0.7269   YZ=    -1.3646   ZZ=    21.6591
Eigenvalues:    21.0833    24.5177    30.3747
  33  H    Isotropic =    26.8858   Anisotropy =    18.3624
```

```
XX=    34.2052   YX=     4.1163   ZX=     6.8970
XY=     6.0389   YY=    27.8244   ZY=    -0.3986
XZ=     7.0650   YZ=     2.0314   ZZ=    18.6279
Eigenvalues:    15.8545    25.6756    39.1274
  34  H    Isotropic =    32.2395   Anisotropy =    17.7175
XX=    43.4046   YX=    -2.3976   ZX=    -2.1496
XY=    -1.8492   YY=    25.8154   ZY=    -1.1198
XZ=    -3.2745   YZ=    -1.4174   ZZ=    27.4987
Eigenvalues:    24.5906    28.0768    44.0512
  35  H    Isotropic =    29.8357   Anisotropy =     7.8951
XX=    34.0593   YX=    -3.3886   ZX=    -0.6849
XY=    -1.0369   YY=    30.2084   ZY=    -1.3186
XZ=    -1.5827   YZ=    -1.0032   ZZ=    25.2395
Eigenvalues:    24.6933    29.7148    35.0991
  36  H    Isotropic =    29.3302   Anisotropy =     8.9229
XX=    30.8226   YX=     3.4914   ZX=     1.4618
XY=     3.1660   YY=    30.4357   ZY=     2.2579
XZ=     2.6327   YZ=     3.1506   ZZ=    26.7322
Eigenvalues:    25.2857    27.4261    35.2787
  37  H    Isotropic =    29.4835   Anisotropy =     8.0776
XX=    30.1113   YX=     1.7202   ZX=    -2.6160
XY=     0.1152   YY=    27.4621   ZY=    -3.6429
XZ=    -2.2428   YZ=    -4.3389   ZZ=    30.8770
Eigenvalues:    24.7580    28.8239    34.8686
  38  H    Isotropic =    29.8711   Anisotropy =     7.9917
XX=    33.5668   YX=     2.1302   ZX=     1.6065
XY=     2.9219   YY=    30.6582   ZY=    -1.0272
XZ=     2.1807   YZ=    -0.4494   ZZ=    25.3884
Eigenvalues:    24.6757    29.7387    35.1989
  39  H    Isotropic =    29.7700   Anisotropy =     4.6092
XX=    26.5927   YX=     0.2806   ZX=    -1.8574
XY=     1.0159   YY=    30.6384   ZY=    -1.0685
XZ=    -2.1378   YZ=     0.4472   ZZ=    32.0789
Eigenvalues:    25.8851    30.5822    32.8428
  40  H    Isotropic =    29.9822   Anisotropy =     8.3460
XX=    28.3742   YX=    -0.3518   ZX=    -0.9311
XY=    -1.6237   YY=    34.8670   ZY=    -1.7602
XZ=    -0.2560   YZ=    -2.7735   ZZ=    26.7053
Eigenvalues:    25.8434    28.5569    35.5462
  41  H    Isotropic =    26.6356   Anisotropy =     5.7311
XX=    27.8748   YX=    -3.2381   ZX=    -1.0002
XY=    -0.4153   YY=    26.5856   ZY=     1.5912
XZ=    -1.1416   YZ=     3.7551   ZZ=    25.4464
Eigenvalues:    23.2566    26.1939    30.4563
  42  H    Isotropic =    26.6539   Anisotropy =     7.0812
XX=    27.1849   YX=    -0.4118   ZX=    -1.2617
XY=    -2.6039   YY=    25.7061   ZY=     4.3004
XZ=    -0.5067   YZ=     4.2514   ZZ=    27.0707
Eigenvalues:    21.9911    26.5959    31.3747
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 45.82 | 60.20 | 76.10 | 87.71 | 102.05 | 160.11 |
| intensities | 0.94 | 0.14 | 1.03 | 0.36 | 1.82 | 1.07 |
| reduc. mass | 0.79 | 0.99 | 0.47 | 1.05 | 1.14 | 0.75 |
| force const | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.01 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 176.06 | 193.18 | 212.89 | 235.94 | 253.13 | 262.19 |
| intensities | 0.43 | 0.27 | 0.66 | 0.43 | 6.93 | 3.94 |
| reduc. mass | 1.29 | 0.74 | 1.32 | 0.64 | 0.99 | 1.25 |
| force const | 0.02 | 0.02 | 0.04 | 0.02 | 0.04 | 0.05 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 271.91 | 281.51 | 302.64 | 307.48 | 315.96 | 341.53 |
| intensities | 4.88 | 4.52 | 1.10 | 1.52 | 0.54 | 6.45 |
| reduc. mass | 0.65 | 0.36 | 0.35 | 0.94 | 0.34 | 1.43 |
| force const | 0.03 | 0.02 | 0.02 | 0.05 | 0.02 | 0.10 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 356.35 | 381.06 | 422.80 | 434.18 | 460.48 | 492.52 |
| intensities | 3.06 | 9.85 | 7.78 | 32.79 | 2.29 | 19.16 |
| reduc. mass | 0.77 | 0.45 | 0.76 | 0.71 | 0.53 | 0.91 |
| force const | 0.06 | 0.04 | 0.08 | 0.08 | 0.07 | 0.13 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 512.44 | 527.08 | 532.23 | 548.18 | 565.05 | 602.16 |
| intensities | 0.68 | 0.43 | 12.07 | 1.72 | 30.10 | 24.03 |
| reduc. mass | 0.57 | 0.74 | 1.77 | 0.64 | 0.56 | 2.49 |
| force const | 0.09 | 0.12 | 0.29 | 0.11 | 0.10 | 0.53 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 634.81 | 666.27 | 675.29 | 694.36 | 718.82 | 736.11 |
| intensities | 102.04 | 9.53 | 11.10 | 8.21 | 2.47 | 10.56 |
| reduc. mass | 0.54 | 0.88 | 1.02 | 1.15 | 0.43 | 0.77 |
| force const | 0.13 | 0.23 | 0.27 | 0.33 | 0.13 | 0.25 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 748.02 | 795.51 | 809.16 | 834.85 | 875.46 | 922.13 |
| intensities | 6.88 | 5.22 | 7.81 | 2.48 | 24.64 | 4.67 |
| reduc. mass | 1.88 | 0.60 | 0.74 | 2.49 | 0.63 | 0.66 |
| force const | 0.62 | 0.22 | 0.28 | 1.02 | 0.28 | 0.33 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 923.23 | 961.60 | 962.94 | 992.39 | 1006.18 | 1021.35 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 12.53 | 6.46 | 8.09 | 3.26 | 1.64 | 7.51 |
| reduc. mass | 0.56 | 0.35 | 1.45 | 0.39 | 0.34 | 0.27 |
| force const | 0.28 | 0.19 | 0.79 | 0.22 | 0.20 | 0.17 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1026.69 | 1044.67 | 1053.62 | 1058.13 | 1063.87 | 1091.57 |
| intensities | 32.44 | 26.69 | 20.64 | 14.05 | 10.97 | 12.50 |
| reduc. mass | 0.29 | 0.36 | 0.41 | 0.23 | 0.24 | 0.44 |
| force const | 0.18 | 0.23 | 0.27 | 0.15 | 0.16 | 0.31 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1100.17 | 1129.84 | 1141.62 | 1161.47 | 1190.34 | 1210.32 |
| intensities | 5.89 | 17.01 | 67.61 | 39.83 | 43.67 | 52.00 |
| reduc. mass | 0.51 | 0.59 | 0.60 | 0.59 | 1.37 | 0.86 |
| force const | 0.37 | 0.44 | 0.46 | 0.47 | 1.14 | 0.74 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1222.96 | 1240.37 | 1250.70 | 1269.63 | 1318.51 | 1329.29 |
| intensities | 31.65 | 102.39 | 43.29 | 63.92 | 93.72 | 31.79 |
| reduc. mass | 0.74 | 0.56 | 0.26 | 0.89 | 0.63 | 0.37 |
| force const | 0.65 | 0.51 | 0.24 | 0.85 | 0.65 | 0.39 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1361.66 | 1398.44 | 1403.22 | 1410.96 | 1424.63 | 1472.90 |
| intensities | 26.47 | 169.34 | 131.93 | 14.94 | 288.28 | 1.49 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.57 | 0.54 | 0.60 | 0.80 | 0.89 | 0.43 |
| force const | 0.62 | 0.63 | 0.69 | 0.94 | 1.06 | 0.54 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1487.58 | 1490.63 | 1511.52 | 1520.94 | 1531.29 | 1542.55 |
| intensities | 4.42 | 9.36 | 183.79 | 33.44 | 36.03 | 4.04 |
| reduc. mass | 0.44 | 0.86 | 1.66 | 2.39 | 0.53 | 0.50 |
| force const | 0.57 | 1.13 | 2.24 | 3.25 | 0.73 | 0.71 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1555.98 | 1567.85 | 1590.00 | 1607.21 | 1635.31 | 1646.00 |
| intensities | 178.89 | 13.16 | 36.59 | 6.19 | 13.05 | 25.26 |
| reduc. mass | 1.21 | 0.77 | 0.96 | 0.72 | 0.71 | 0.56 |
| force const | 1.73 | 1.12 | 1.42 | 1.10 | 1.12 | 0.89 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1648.14 | 1655.87 | 1658.82 | 1662.34 | 1664.80 | 1667.02 |
| intensities | 105.24 | 9.56 | 7.79 | 81.07 | 24.01 | 1.84 |
| reduc. mass | 0.52 | 0.34 | 0.39 | 0.26 | 0.32 | 0.35 |
| force const | 0.83 | 0.56 | 0.64 | 0.42 | 0.52 | 0.57 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1669.13 | 1672.30 | 1684.96 | 1686.48 | 1723.50 | 1802.41 |
| intensities | 9.47 | 10.71 | 33.06 | 88.12 | 39.77 | 830.80 |
| reduc. mass | 0.17 | 0.38 | 0.26 | 0.77 | 1.04 | 1.47 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 0.29 | 0.62 | 0.44 | 1.29 | 1.82 | 2.82 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1838.89 | 1889.59 | 3022.62 | 3023.91 | 3036.90 | 3050.77 |
| intensities | 394.83 | 11.08 | 467.86 | 249.05 | 641.12 | 487.25 |
| reduc. mass | 1.39 | 0.85 | 0.29 | 0.29 | 0.30 | 0.47 |
| force const | 2.77 | 1.80 | 1.57 | 1.55 | 1.65 | 2.56 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3057.90 | 3074.39 | 3081.82 | 3091.82 | 3101.53 | 3118.80 |
| intensities | 607.49 | 472.77 | 150.21 | 442.73 | 197.37 | 449.47 |
| reduc. mass | 0.45 | 0.92 | 0.80 | 0.47 | 0.82 | 0.52 |
| force const | 2.48 | 5.11 | 4.50 | 2.64 | 4.64 | 3.00 |

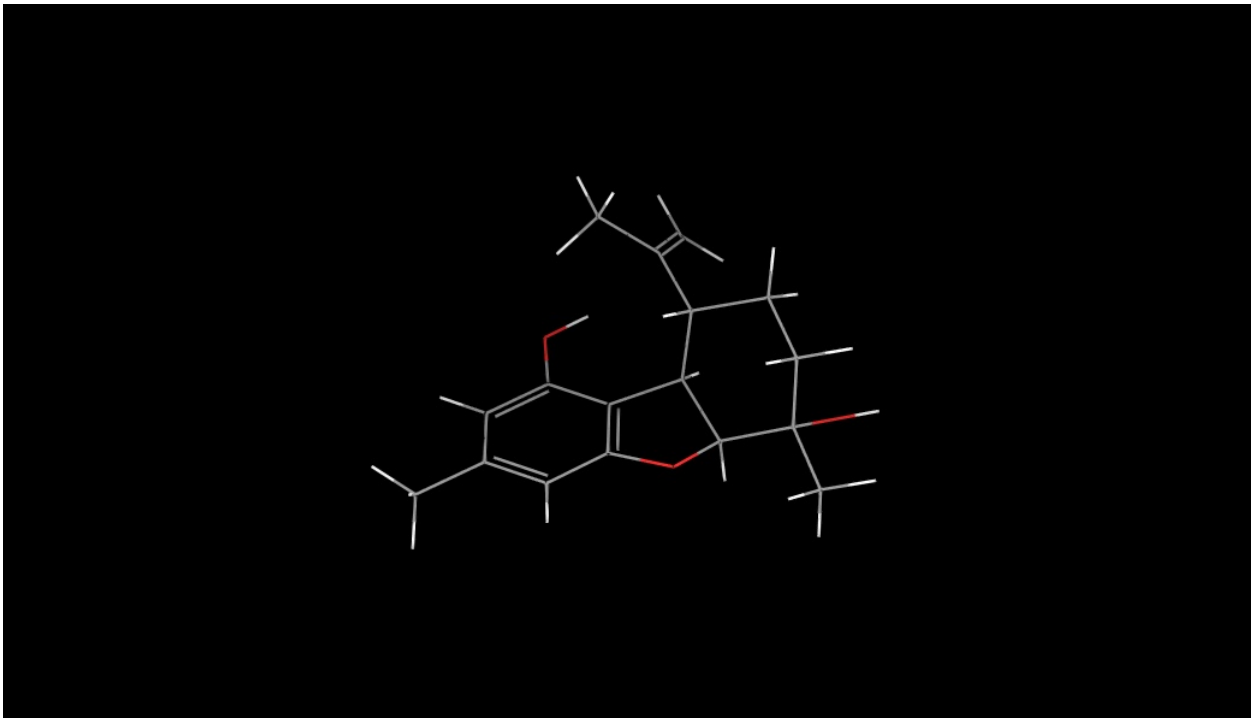
| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3126.25 | 3129.52 | 3135.89 | 3137.29 | 3145.64 | 3146.93 |
| intensities | 297.33 | 454.75 | 272.49 | 689.92 | 413.62 | 109.51 |
| reduc. mass | 0.42 | 0.42 | 0.28 | 0.28 | 0.53 | 0.46 |
| force const | 2.42 | 2.42 | 1.62 | 1.65 | 3.07 | 2.69 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3149.34 | 3153.39 | 3156.72 | 3195.82 | 3842.11 | 3849.28 |
| intensities | 307.66 | 543.28 | 228.75 | 311.19 | 70.39 | 116.45 |
| reduc. mass | 0.54 | 0.73 | 0.83 | 0.56 | 0.93 | 0.93 |
| force const | 3.15 | 4.27 | 4.87 | 3.36 | 8.05 | 8.09 |

Number of imaginary frequencies:

Conformation 2

Boltzmann Population = 24.3% (relative energy = 0.32 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.983588 hartrees

Total enthalpy, Htot (Utot + pV): -885.982644 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.044700 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.052500 | -0.656100 | -2.563700 |
| 2 | 6 | 0 | -4.588400 | -0.353100 | -2.877300 |
| 3 | 6 | 0 | -3.893800 | -1.630700 | -3.360200 |
| 4 | 6 | 0 | -3.972400 | -2.755800 | -2.299100 |

| | | | | | |
|---|---|---|---|---|---|
| 5 | 6 | 0 | -5.385400 | -2.948100 | -1.718600 |
| 6 | 6 | 0 | -6.178700 | -1.675800 | -1.427000 |
| 7 | 6 | 0 | -7.635300 | -2.008400 | -1.126000 |
| 8 | 6 | 0 | -2.454700 | -1.412000 | -3.797900 |
| 9 | 6 | 0 | -3.817600 | -4.099100 | -2.976300 |
| 10 | 6 | 0 | -5.103300 | -4.589100 | -3.214000 |
| 11 | 6 | 0 | -2.729500 | -4.780300 | -3.502900 |
| 12 | 6 | 0 | -2.955600 | -5.961900 | -4.223200 |
| 13 | 6 | 0 | -4.246100 | -6.436100 | -4.440900 |
| 14 | 6 | 0 | -5.354600 | -5.739400 | -3.934300 |
| 15 | 8 | 0 | -1.446900 | -4.356000 | -3.367700 |
| 16 | 8 | 0 | -6.069000 | -3.782000 | -2.670600 |
| 17 | 8 | 0 | -5.531100 | -1.174900 | -0.257300 |
| 18 | 6 | 0 | -4.469000 | -7.712600 | -5.212900 |
| 19 | 6 | 0 | -2.148900 | -1.716800 | -5.237900 |
| 20 | 6 | 0 | -1.518500 | -0.990800 | -2.940800 |
| 21 | 1 | 0 | -6.555100 | -1.053100 | -3.454300 |
| 22 | 1 | 0 | -6.589800 | 0.256800 | -2.274600 |
| 23 | 1 | 0 | -4.509200 | 0.421300 | -3.647400 |
| 24 | 1 | 0 | -4.090900 | 0.025500 | -1.977900 |
| 25 | 1 | 0 | -4.457700 | -1.988700 | -4.232900 |
| 26 | 1 | 0 | -3.262400 | -2.558500 | -1.490200 |
| 27 | 1 | 0 | -5.307000 | -3.508600 | -0.776100 |
| 28 | 1 | 0 | -8.179600 | -1.096100 | -0.857300 |
| 29 | 1 | 0 | -8.118700 | -2.459700 | -1.994500 |
| 30 | 1 | 0 | -7.693900 | -2.707300 | -0.287400 |
| 31 | 1 | 0 | -2.095400 | -6.491700 | -4.618800 |
| 32 | 1 | 0 | -6.368500 | -6.089000 | -4.094200 |
| 33 | 1 | 0 | -1.441200 | -3.460600 | -2.997500 |
| 34 | 1 | 0 | -5.981200 | -0.361400 | 0.000900 |
| 35 | 1 | 0 | -3.554500 | -8.041500 | -5.710300 |
| 36 | 1 | 0 | -4.799300 | -8.516600 | -4.547700 |
| 37 | 1 | 0 | -5.244000 | -7.579300 | -5.973100 |
| 38 | 1 | 0 | -2.762400 | -1.089500 | -5.894700 |
| 39 | 1 | 0 | -1.096400 | -1.550900 | -5.477200 |
| 40 | 1 | 0 | -2.401300 | -2.759400 | -5.464100 |
| 41 | 1 | 0 | -0.493000 | -0.829700 | -3.259300 |
| 42 | 1 | 0 | -1.751800 | -0.769200 | -1.902400 |

---

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 147.6671 Anisotropy = 22.0578

XX= 142.7813 YX= -1.7247 ZX= 3.0509

XY= -7.5685 YY= 154.4948 ZY= 9.4693

XZ= -4.0115 YZ= 11.5359 ZZ= 145.7252

Eigenvalues: 137.6547 142.9743 162.3723

2 C Isotropic = 157.9013 Anisotropy = 23.2390

XX= 166.6189 YX= -8.2506 ZX= 6.4787

XY= -3.1470 YY= 160.4962 ZY= -6.4401

XZ= 7.7887 YZ= -6.5681 ZZ= 146.5890

Eigenvalues: 143.0134 157.2965 173.3940

```
   3  C    Isotropic =   135.8122   Anisotropy =    11.2599
XX=   141.3005   YX=    -3.8254   ZX=    -0.5061
XY=     8.5788   YY=   140.3025   ZY=    -3.3502
XZ=     6.6421   YZ=    -7.2157   ZZ=   125.8337
Eigenvalues:   123.3620   140.7559   143.3188
   4  C    Isotropic =   135.8645   Anisotropy =    28.3604
XX=   127.0381   YX=     4.8436   ZX=     2.0517
XY=     3.4601   YY=   151.7713   ZY=    -3.4354
XZ=     7.5567   YZ=    17.4674   ZZ=   128.7840
Eigenvalues:   122.9512   129.8707   154.7714
   5  C    Isotropic =    97.3788   Anisotropy =    57.0800
XX=   117.8137   YX=    11.8011   ZX=   -19.2985
XY=     3.8964   YY=    92.6681   ZY=   -23.4052
XZ=   -27.4683   YZ=   -15.5287   ZZ=    81.6545
Eigenvalues:    62.7053    93.9989   135.4321
   6  C    Isotropic =   115.5928   Anisotropy =    54.2499
XX=   114.1450   YX=    11.8572   ZX=   -29.8773
XY=     8.5601   YY=   111.1503   ZY=   -10.5964
XZ=   -26.0036   YZ=   -12.2000   ZZ=   121.4831
Eigenvalues:    89.6323   105.3867   151.7594
   7  C    Isotropic =   157.6089   Anisotropy =    44.8854
XX=   145.4052   YX=   -11.8846   ZX=     1.2116
XY=    -7.5161   YY=   184.7111   ZY=    -4.3113
XZ=    -0.6472   YZ=    -5.8236   ZZ=   142.7103
Eigenvalues:   141.6453   143.6489   187.5324
   8  C    Isotropic =    16.8506   Anisotropy =   212.3856
XX=    42.1418   YX=    81.2167   ZX=   101.5621
XY=    83.3703   YY=   -28.0805   ZY=    -5.2563
XZ=    96.9746   YZ=     2.9721   ZZ=    36.4906
Eigenvalues:  -109.7472     1.8580   158.4411
   9  C    Isotropic =    68.1335   Anisotropy =   109.7793
XX=    23.8231   YX=    -1.7045   ZX=     8.6870
XY=   -16.7931   YY=    60.0124   ZY=    38.9722
XZ=    15.0092   YZ=    42.2939   ZZ=   120.5651
Eigenvalues:    15.7602    47.3207   141.3198
  10  C    Isotropic =    20.7575   Anisotropy =   110.1366
XX=   -32.3950   YX=    33.5083   ZX=    -4.6388
XY=    43.5082   YY=    11.9417   ZY=    35.8827
XZ=   -16.4881   YZ=    25.1622   ZZ=    82.7258
Eigenvalues:   -59.0154    27.1060    94.1819
  11  C    Isotropic =    28.0795   Anisotropy =   135.4805
XX=    14.8724   YX=    -6.4604   ZX=    10.2551
XY=    -0.5721   YY=   -26.0746   ZY=    61.1438
XZ=     6.8151   YZ=    52.7970   ZZ=    95.4408
Eigenvalues:   -49.2495    15.0882   118.3999
  12  C    Isotropic =    74.3263   Anisotropy =   114.4930
XX=    21.3712   YX=    31.1989   ZX=    -3.7848
XY=    42.0269   YY=    62.5391   ZY=    35.9609
XZ=    -3.8124   YZ=    25.9274   ZZ=   139.0687
Eigenvalues:    -2.7006    75.0247   150.6550
  13  C    Isotropic =    41.3562   Anisotropy =   193.5352
XX=   -40.7816   YX=   -15.3216   ZX=    22.9869
```

```
XY=   -18.2033   YY=    29.7066   ZY=    66.7232
XZ=    29.9820   YZ=    70.8537   ZZ=   135.1435
Eigenvalues:   -55.8383     9.5271   170.3796
  14  C    Isotropic =    81.5049   Anisotropy =   122.6674
XX=    74.4386   YX=    10.2735   ZX=     2.9895
XY=    -6.4322   YY=    33.3274   ZY=    60.7925
XZ=     5.6428   YZ=    55.9817   ZZ=   136.7488
Eigenvalues:     7.0442    74.1874   163.2832
  15  O    Isotropic =   202.8368   Anisotropy =    76.1666
XX=   147.0906   YX=    13.6827   ZX=     0.6158
XY=     6.5367   YY=   210.9614   ZY=    10.4376
XZ=    24.6111   YZ=   -29.4833   ZZ=   250.4585
Eigenvalues:   143.6997   211.1962   253.6146
  16  O    Isotropic =   189.2698   Anisotropy =   117.7058
XX=   224.5859   YX=   -61.5407   ZX=    35.4855
XY=   -47.4961   YY=   157.0777   ZY=    30.5299
XZ=    34.9904   YZ=   -35.4582   ZZ=   186.1457
Eigenvalues:   122.6761   177.3929   267.7403
  17  O    Isotropic =   247.2430   Anisotropy =    93.5963
XX=   308.6738   YX=    11.6473   ZX=   -15.3188
XY=     4.0421   YY=   200.5081   ZY=    -5.8176
XZ=     5.3856   YZ=   -10.4483   ZZ=   232.5473
Eigenvalues:   198.1783   233.9102   309.6406
  18  C    Isotropic =   163.8385   Anisotropy =    41.4833
XX=   186.0189   YX=     6.8138   ZX=    -9.3712
XY=    12.9253   YY=   157.8903   ZY=    -9.2121
XZ=    -6.8841   YZ=    -6.3503   ZZ=   147.6063
Eigenvalues:   143.2425   156.7791   191.4941
  19  C    Isotropic =   157.9626   Anisotropy =    42.5385
XX=   158.9190   YX=   -15.3714   ZX=   -17.3422
XY=   -12.0723   YY=   159.8984   ZY=     8.8407
XZ=   -18.9870   YZ=    11.7281   ZZ=   155.0703
Eigenvalues:   138.5533   149.0129   186.3215
  20  C    Isotropic =    72.1357   Anisotropy =   131.0835
XX=    89.0191   YX=    76.8064   ZX=    48.7645
XY=    72.9334   YY=    24.8007   ZY=   -15.9101
XZ=    49.7865   YZ=   -18.2457   ZZ=   102.5873
Eigenvalues:   -37.3166    94.1990   159.5247
  21  H    Isotropic =    29.9890   Anisotropy =     6.0700
XX=    27.4460   YX=    -0.7828   ZX=    -0.8749
XY=     0.1276   YY=    28.9965   ZY=    -1.4198
XZ=     0.3728   YZ=    -1.7794   ZZ=    33.5246
Eigenvalues:    27.3146    28.6168    34.0357
  22  H    Isotropic =    30.4436   Anisotropy =     8.5245
XX=    33.5581   YX=    -2.2351   ZX=     3.8968
XY=    -1.7921   YY=    29.7424   ZY=     0.2831
XZ=     4.1466   YZ=     0.1422   ZZ=    28.0303
Eigenvalues:    25.5872    29.6170    36.1265
  23  H    Isotropic =    30.4381   Anisotropy =     9.5373
XX=    29.9690   YX=     0.6546   ZX=     3.9574
XY=     0.9585   YY=    31.1689   ZY=     4.4741
XZ=     4.3209   YZ=     4.0852   ZZ=    30.1764
```

```
Eigenvalues:    24.7711    29.7469    36.7963
  24  H    Isotropic =    29.8180   Anisotropy =     5.8030
XX=    30.8420   YX=     1.3110   ZX=    -2.6321
XY=     1.5127   YY=    31.5530   ZY=    -1.8301
XZ=    -1.7811   YZ=    -1.2876   ZZ=    27.0589
Eigenvalues:    25.9079    29.8593    33.6866
  25  H    Isotropic =    30.1302   Anisotropy =     3.7995
XX=    30.8205   YX=    -1.7091   ZX=    -2.3344
XY=    -0.1903   YY=    29.7859   ZY=     0.5566
XZ=     0.0515   YZ=     2.8216   ZZ=    29.7842
Eigenvalues:    28.0871    29.6403    32.6632
  26  H    Isotropic =    28.5622   Anisotropy =     4.5451
XX=    27.3206   YX=    -0.0943   ZX=     0.0568
XY=    -1.7865   YY=    29.1857   ZY=    -2.1112
XZ=    -0.9610   YZ=    -2.6485   ZZ=    29.1803
Eigenvalues:    26.0358    28.0585    31.5922
  27  H    Isotropic =    27.6230   Anisotropy =     4.9297
XX=    26.8061   YX=     0.6798   ZX=    -1.1596
XY=    -1.1137   YY=    27.4223   ZY=     0.9060
XZ=    -3.1260   YZ=     2.8657   ZZ=    28.6407
Eigenvalues:    24.9969    26.9627    30.9095
  28  H    Isotropic =    30.9536   Anisotropy =     8.8686
XX=    33.7492   YX=    -3.1143   ZX=     1.7862
XY=    -4.3521   YY=    31.3856   ZY=    -0.8075
XZ=     1.7936   YZ=    -0.6268   ZZ=    27.7262
Eigenvalues:    27.1933    28.8016    36.8660
  29  H    Isotropic =    29.9853   Anisotropy =     8.3508
XX=    29.2262   YX=     0.0357   ZX=    -1.8226
XY=     0.5722   YY=    32.3233   ZY=    -4.7871
XZ=    -1.8064   YZ=    -4.2686   ZZ=    28.4063
Eigenvalues:    24.9860    29.4173    35.5525
  30  H    Isotropic =    30.3310   Anisotropy =     9.0934
XX=    27.9468   YX=    -1.1015   ZX=    -0.0413
XY=    -1.0241   YY=    34.0540   ZY=     4.6808
XZ=    -0.0370   YZ=     3.3897   ZZ=    28.9922
Eigenvalues:    26.5789    28.0207    36.3933
  31  H    Isotropic =    25.3006   Anisotropy =     6.6714
XX=    27.0913   YX=     2.2731   ZX=    -0.9506
XY=     2.5069   YY=    26.2822   ZY=    -2.2792
XZ=    -0.6595   YZ=    -2.3322   ZZ=    22.5282
Eigenvalues:    21.4128    24.7408    29.7481
  32  H    Isotropic =    25.3702   Anisotropy =     7.4452
XX=    30.1452   YX=     0.4609   ZX=    -0.7902
XY=     0.9546   YY=    24.1967   ZY=    -1.2735
XZ=    -0.7729   YZ=    -1.4665   ZZ=    21.7688
Eigenvalues:    21.1319    24.6451    30.3337
  33  H    Isotropic =    26.4630   Anisotropy =    16.8420
XX=    35.2212   YX=     4.1769   ZX=     3.3059
XY=     6.0480   YY=    26.1854   ZY=    -2.7305
XZ=     2.0190   YZ=    -0.4049   ZZ=    17.9825
Eigenvalues:    16.9142    24.7838    37.6911
  34  H    Isotropic =    32.2093   Anisotropy =    17.5947
```

```
XX=    43.6564   YX=    -0.1200   ZX=    -1.5531
XY=     0.4593   YY=    25.2274   ZY=    -1.1773
XZ=    -2.6768   YZ=    -1.5777   ZZ=    27.7442
Eigenvalues:    24.5929    28.0959    43.9391
  35  H    Isotropic =    29.8512   Anisotropy =     7.8672
XX=    34.3479   YX=    -3.1160   ZX=    -0.5179
XY=    -0.7700   YY=    29.8366   ZY=    -1.5440
XZ=    -1.5816   YZ=    -1.2559   ZZ=    25.3692
Eigenvalues:    24.7068    29.7508    35.0961
  36  H    Isotropic =    29.3315   Anisotropy =     8.9891
XX=    30.4422   YX=     3.6315   ZX=     1.0997
XY=     3.2891   YY=    31.1924   ZY=     2.1204
XZ=     2.1995   YZ=     3.0559   ZZ=    26.3600
Eigenvalues:    25.2298    27.4406    35.3243
  37  H    Isotropic =    29.4704   Anisotropy =     8.0710
XX=    29.8966   YX=     1.7341   ZX=    -2.4008
XY=     0.2044   YY=    27.2116   ZY=    -3.5882
XZ=    -1.9825   YZ=    -4.3201   ZZ=    31.3031
Eigenvalues:    24.7837    28.7765    34.8511
  38  H    Isotropic =    30.0529   Anisotropy =     7.9614
XX=    27.4007   YX=    -0.8187   ZX=     0.6443
XY=    -1.0935   YY=    28.4032   ZY=     2.7540
XZ=     1.0738   YZ=     2.4513   ZZ=    34.3547
Eigenvalues:    26.2038    28.5943    35.3605
  39  H    Isotropic =    29.9826   Anisotropy =     8.7694
XX=    28.1900   YX=    -3.7264   ZX=    -0.7346
XY=    -2.1380   YY=    34.3453   ZY=    -0.1039
XZ=    -1.3738   YZ=     2.7361   ZZ=    27.4124
Eigenvalues:    26.5765    27.5425    35.8289
  40  H    Isotropic =    29.9857   Anisotropy =     5.6913
XX=    32.3157   YX=     2.3642   ZX=    -1.3434
XY=     1.8119   YY=    30.0870   ZY=     2.3128
XZ=    -0.2722   YZ=     4.0572   ZZ=    27.5542
Eigenvalues:    24.9207    31.2564    33.7799
  41  H    Isotropic =    26.3562   Anisotropy =     5.5294
XX=    25.2986   YX=     3.0941   ZX=    -1.1331
XY=     1.1238   YY=    27.4965   ZY=    -1.2261
XZ=     0.1575   YZ=    -3.2316   ZZ=    26.2736
Eigenvalues:    23.6917    25.3345    30.0425
  42  H    Isotropic =    26.3123   Anisotropy =     8.1556
XX=    24.8889   YX=     0.7231   ZX=     0.3516
XY=     3.3779   YY=    28.2573   ZY=    -5.9205
XZ=    -0.7613   YZ=    -2.2367   ZZ=    25.7908
Eigenvalues:    22.2705    24.9171    31.7494
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 59.14 | 87.68 | 94.71 | 109.12 | 126.58 | 138.04 |
| intensities | 0.61 | 0.25 | 1.41 | 0.83 | 0.79 | 3.02 |
| reduc. mass | 1.40 | 0.84 | 1.09 | 1.32 | 0.28 | 1.29 |
| force const | 0.00 | 0.00 | 0.01 | 0.01 | 0.00 | 0.01 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 165.66 | 192.76 | 222.97 | 246.86 | 253.37 | 266.47 |
| intensities | 0.69 | 0.55 | 1.10 | 0.95 | 6.21 | 6.14 |
| reduc. mass | 0.73 | 0.76 | 1.48 | 0.68 | 0.71 | 1.31 |
| force const | 0.01 | 0.02 | 0.04 | 0.02 | 0.03 | 0.05 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 268.27 | 294.19 | 298.92 | 305.26 | 314.60 | 343.16 |
| intensities | 0.58 | 3.40 | 1.43 | 0.96 | 0.27 | 7.97 |
| reduc. mass | 0.89 | 0.27 | 1.24 | 0.32 | 0.30 | 1.35 |
| force const | 0.04 | 0.01 | 0.07 | 0.02 | 0.02 | 0.09 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 354.19 | 401.20 | 420.57 | 450.34 | 470.29 | 495.73 |
| intensities | 4.34 | 1.78 | 6.41 | 2.54 | 20.86 | 10.94 |
| reduc. mass | 0.77 | 0.55 | 0.49 | 0.68 | 0.51 | 0.79 |
| force const | 0.06 | 0.05 | 0.05 | 0.08 | 0.07 | 0.11 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 520.48 | 524.23 | 543.65 | 556.16 | 565.43 | 602.39 |
| intensities | 8.82 | 13.83 | 3.00 | 23.71 | 43.32 | 25.99 |
| reduc. mass | 0.47 | 2.09 | 0.53 | 0.56 | 0.49 | 2.16 |
| force const | 0.08 | 0.34 | 0.09 | 0.10 | 0.09 | 0.46 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 649.40 | 664.05 | 691.94 | 706.41 | 709.52 | 717.73 |
| intensities | 79.81 | 29.64 | 9.15 | 5.34 | 15.29 | 3.07 |
| reduc. mass | 0.49 | 0.76 | 1.11 | 0.82 | 0.91 | 0.36 |
| force const | 0.12 | 0.20 | 0.31 | 0.24 | 0.27 | 0.11 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 746.37 | 807.49 | 819.33 | 851.15 | 872.10 | 932.41 |
| intensities | 16.03 | 1.86 | 4.63 | 6.03 | 12.20 | 3.30 |
| reduc. mass | 0.73 | 0.99 | 1.84 | 0.75 | 0.61 | 0.75 |
| force const | 0.24 | 0.38 | 0.73 | 0.32 | 0.27 | 0.39 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 938.22 | 951.95 | 956.96 | 988.32 | 1010.25 | 1016.16 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 3.48 | 23.22 | 16.52 | 9.79 | 0.43 | 14.85 |
| reduc. mass | 0.45 | 0.98 | 0.31 | 0.30 | 0.22 | 0.28 |
| force const | 0.24 | 0.52 | 0.17 | 0.17 | 0.13 | 0.17 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1030.16 | 1046.38 | 1050.01 | 1054.22 | 1056.75 | 1093.60 |
| intensities | 23.64 | 2.86 | 24.94 | 4.21 | 33.93 | 8.92 |
| reduc. mass | 0.50 | 0.55 | 0.34 | 0.26 | 0.31 | 0.60 |
| force const | 0.31 | 0.35 | 0.22 | 0.17 | 0.20 | 0.43 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1113.28 | 1132.88 | 1143.29 | 1153.81 | 1164.77 | 1210.00 |
| intensities | 28.74 | 8.16 | 6.58 | 53.68 | 54.09 | 14.54 |
| reduc. mass | 0.39 | 0.56 | 0.44 | 0.71 | 0.36 | 0.32 |
| force const | 0.29 | 0.42 | 0.34 | 0.56 | 0.28 | 0.28 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1215.04 | 1228.28 | 1253.56 | 1259.29 | 1305.87 | 1321.46 |
| intensities | 108.41 | 27.30 | 65.38 | 51.58 | 43.68 | 90.20 |
| reduc. mass | 1.20 | 0.56 | 0.40 | 0.37 | 0.67 | 0.53 |
| force const | 1.04 | 0.49 | 0.37 | 0.35 | 0.67 | 0.54 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1366.62 | 1400.37 | 1401.62 | 1422.62 | 1435.28 | 1484.26 |
| intensities | 24.04 | 215.51 | 146.05 | 201.90 | 88.15 | 10.81 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.51 | 0.44 | 0.30 | 1.15 | 0.52 | 1.44 |
| force const | 0.56 | 0.51 | 0.35 | 1.37 | 0.63 | 1.87 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1497.21 | 1505.56 | 1512.09 | 1513.98 | 1526.13 | 1531.11 |
| intensities | 7.14 | 29.86 | 77.59 | 82.28 | 23.13 | 59.43 |
| reduc. mass | 0.62 | 0.64 | 1.00 | 0.86 | 0.94 | 0.72 |
| force const | 0.82 | 0.85 | 1.35 | 1.16 | 1.29 | 1.00 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1540.40 | 1566.52 | 1587.60 | 1617.72 | 1629.26 | 1632.44 |
| intensities | 36.95 | 120.02 | 18.07 | 57.25 | 50.98 | 53.63 |
| reduc. mass | 0.57 | 0.97 | 0.52 | 0.26 | 0.23 | 0.38 |
| force const | 0.79 | 1.41 | 0.78 | 0.40 | 0.35 | 0.60 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1641.26 | 1649.60 | 1656.06 | 1658.48 | 1660.43 | 1665.29 |
| intensities | 6.60 | 29.31 | 33.09 | 72.18 | 12.61 | 2.85 |
| reduc. mass | 0.52 | 1.04 | 0.13 | 0.37 | 0.34 | 0.35 |
| force const | 0.83 | 1.67 | 0.20 | 0.60 | 0.56 | 0.57 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1669.60 | 1670.15 | 1672.21 | 1687.26 | 1687.79 | 1803.55 |
| intensities | 18.74 | 6.85 | 14.40 | 78.99 | 24.19 | 854.83 |
| reduc. mass | 0.13 | 0.27 | 0.24 | 0.55 | 0.38 | 1.63 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 0.21 | 0.44 | 0.40 | 0.93 | 0.64 | 3.12 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1834.94 | 1889.25 | 3019.05 | 3023.29 | 3028.79 | 3049.45 |
| intensities | 370.85 | 20.27 | 233.88 | 490.19 | 587.60 | 564.50 |
| reduc. mass | 1.35 | 0.87 | 0.30 | 0.31 | 0.31 | 0.45 |
| force const | 2.68 | 1.83 | 1.63 | 1.67 | 1.67 | 2.47 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3057.36 | 3076.42 | 3077.12 | 3104.37 | 3106.12 | 3117.91 |
| intensities | 738.73 | 340.33 | 155.88 | 386.97 | 80.28 | 507.92 |
| reduc. mass | 0.42 | 0.83 | 0.68 | 0.35 | 0.27 | 0.44 |
| force const | 2.32 | 4.64 | 3.80 | 1.97 | 1.52 | 2.53 |

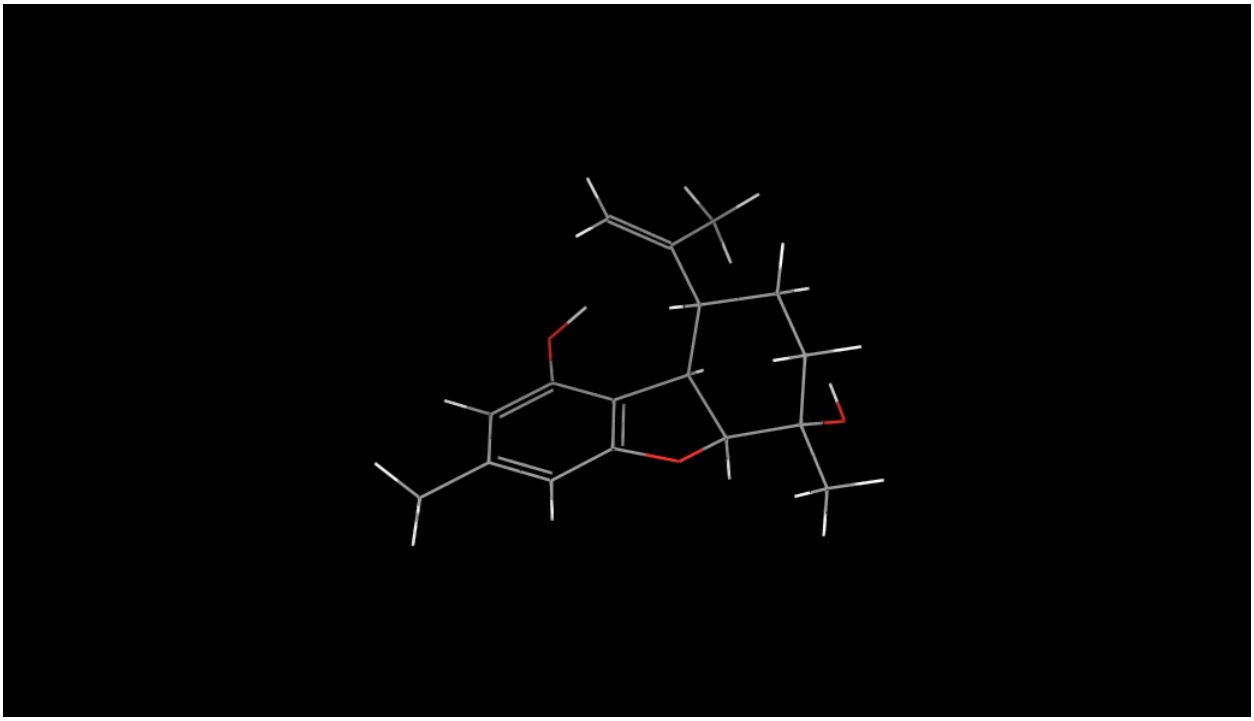
| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3125.57 | 3130.48 | 3135.57 | 3138.04 | 3145.35 | 3148.29 |
| intensities | 386.03 | 135.46 | 447.48 | 628.84 | 575.20 | 78.91 |
| reduc. mass | 0.47 | 0.43 | 0.46 | 0.47 | 0.29 | 0.26 |
| force const | 2.69 | 2.48 | 2.69 | 2.72 | 1.67 | 1.53 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3152.63 | 3154.56 | 3164.94 | 3195.81 | 3826.30 | 3851.07 |
| intensities | 172.89 | 554.20 | 120.91 | 330.36 | 78.65 | 131.86 |
| reduc. mass | 0.35 | 0.48 | 0.59 | 0.56 | 0.95 | 0.95 |
| force const | 2.06 | 2.79 | 3.48 | 3.36 | 8.15 | 8.26 |

Number of imaginary frequencies: 0

Conformation 3

Boltzmann Population = 1.1% (relative energy = 2.13 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.979047 hartrees

Total enthalpy, Htot (Utot + pV): -885.978103 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.040405 hartrees

Optimized geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.138600 | -0.662600 | -2.587900 |
| 2 | 6 | 0 | -4.679300 | -0.333500 | -2.898000 |
| 3 | 6 | 0 | -3.930700 | -1.587100 | -3.369700 |

| | | | | | |
|---|---|---|---|---|---|
| 4 | 6 | 0 | -4.019800 | -2.748800 | -2.338400 |
| 5 | 6 | 0 | -5.447500 | -2.949100 | -1.772600 |
| 6 | 6 | 0 | -6.253300 | -1.687700 | -1.456300 |
| 7 | 6 | 0 | -7.703000 | -2.040100 | -1.166500 |
| 8 | 6 | 0 | -2.485200 | -1.311600 | -3.730600 |
| 9 | 6 | 0 | -3.865100 | -4.090400 | -3.028000 |
| 10 | 6 | 0 | -5.150100 | -4.572400 | -3.279600 |
| 11 | 6 | 0 | -2.776800 | -4.824100 | -3.486900 |
| 12 | 6 | 0 | -3.007400 | -6.026200 | -4.165700 |
| 13 | 6 | 0 | -4.300800 | -6.485100 | -4.407700 |
| 14 | 6 | 0 | -5.405000 | -5.745100 | -3.964300 |
| 15 | 8 | 0 | -1.485300 | -4.446700 | -3.287700 |
| 16 | 8 | 0 | -6.116400 | -3.754400 | -2.758500 |
| 17 | 8 | 0 | -5.739400 | -1.148500 | -0.240900 |
| 18 | 6 | 0 | -4.516600 | -7.797700 | -5.118900 |
| 19 | 6 | 0 | -1.670100 | -0.489400 | -2.763400 |
| 20 | 6 | 0 | -1.953600 | -1.796200 | -4.856600 |
| 21 | 1 | 0 | -6.620300 | -1.071900 | -3.484000 |
| 22 | 1 | 0 | -6.687800 | 0.236900 | -2.292000 |
| 23 | 1 | 0 | -4.615900 | 0.436200 | -3.674700 |
| 24 | 1 | 0 | -4.196200 | 0.099000 | -2.010500 |
| 25 | 1 | 0 | -4.441700 | -1.942900 | -4.273400 |
| 26 | 1 | 0 | -3.304100 | -2.594400 | -1.520800 |
| 27 | 1 | 0 | -5.380200 | -3.540200 | -0.847800 |
| 28 | 1 | 0 | -8.177300 | -2.470400 | -2.050000 |
| 29 | 1 | 0 | -8.240200 | -1.137700 | -0.863700 |
| 30 | 1 | 0 | -7.753500 | -2.764000 | -0.349100 |
| 31 | 1 | 0 | -2.145600 | -6.588800 | -4.509800 |
| 32 | 1 | 0 | -6.421900 | -6.082200 | -4.130700 |
| 33 | 1 | 0 | -1.458800 | -3.483200 | -3.211100 |
| 34 | 1 | 0 | -4.811200 | -0.921200 | -0.369500 |
| 35 | 1 | 0 | -3.704500 | -8.006600 | -5.818900 |
| 36 | 1 | 0 | -4.557600 | -8.624700 | -4.402100 |
| 37 | 1 | 0 | -5.457600 | -7.795000 | -5.674100 |
| 38 | 1 | 0 | -2.009800 | 0.551700 | -2.754800 |
| 39 | 1 | 0 | -1.762900 | -0.860300 | -1.735600 |
| 40 | 1 | 0 | -0.612200 | -0.496400 | -3.033800 |
| 41 | 1 | 0 | -0.911900 | -1.625900 | -5.114100 |
| 42 | 1 | 0 | -2.546800 | -2.383000 | -5.552200 |

---

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 151.6546 Anisotropy = 19.3622

XX= 146.3294 YX= 0.5986 ZX= 3.4848

XY= -4.8641 YY= 156.1403 ZY= 10.0703

XZ= -3.2345 YZ= 9.8216 ZZ= 152.4941

Eigenvalues: 143.4364 146.9645 164.5627

2 C Isotropic = 161.2063 Anisotropy = 18.9410

XX= 167.0311 YX= -7.1969 ZX= 6.9720

XY= -5.5485 YY= 160.8185 ZY= -1.3494

XZ= 8.2150 YZ= -0.8611 ZZ= 155.7693

```
Eigenvalues:   151.4683   158.3169   173.8336
   3  C    Isotropic =   134.9454   Anisotropy =    15.0877
XX=   136.4137   YX=    -1.3796   ZX=     2.1056
XY=     6.4706   YY=   140.8074   ZY=    -6.4409
XZ=     0.5099   YZ=    -9.7184   ZZ=   127.6150
Eigenvalues:   123.3802   136.4520   145.0038
   4  C    Isotropic =   142.3232   Anisotropy =    21.3732
XX=   147.8293   YX=     0.0545   ZX=     1.8652
XY=     2.0064   YY=   148.1992   ZY=     1.9495
XZ=     7.9845   YZ=    24.3557   ZZ=   130.9410
Eigenvalues:   123.2306   147.1669   156.5719
   5  C    Isotropic =    95.5535   Anisotropy =    59.8365
XX=   120.0521   YX=    10.2379   ZX=   -23.9270
XY=    -1.7573   YY=    86.9351   ZY=   -19.3840
XZ=   -28.4132   YZ=   -12.4082   ZZ=    79.6731
Eigenvalues:    60.5949    90.6211   135.4444
   6  C    Isotropic =   116.7303   Anisotropy =    54.7650
XX=   120.4044   YX=    12.6973   ZX=   -28.1403
XY=    10.2505   YY=   106.9532   ZY=   -10.3451
XZ=   -24.3362   YZ=   -11.2748   ZZ=   122.8332
Eigenvalues:    95.2531   101.6975   153.2403
   7  C    Isotropic =   161.0242   Anisotropy =    40.6170
XX=   147.6448   YX=    -7.2915   ZX=    -0.0638
XY=    -4.3695   YY=   187.2248   ZY=    -0.5249
XZ=    -0.4840   YZ=    -1.9890   ZZ=   148.2030
Eigenvalues:   146.6684   148.3020   188.1022
   8  C    Isotropic =    29.4637   Anisotropy =   191.1253
XX=    61.2560   YX=    -9.3752   ZX=    76.8258
XY=   -16.1357   YY=   -50.7386   ZY=    66.1609
XZ=    79.1664   YZ=    67.2339   ZZ=    77.8736
Eigenvalues:   -92.6544    24.1649   156.8805
   9  C    Isotropic =    66.9265   Anisotropy =   110.0639
XX=    19.3819   YX=     2.7535   ZX=     8.5829
XY=   -12.7999   YY=    61.8413   ZY=    36.6998
XZ=    22.3382   YZ=    41.2333   ZZ=   119.5562
Eigenvalues:    13.7232    46.7538   140.3024
  10  C    Isotropic =    20.5228   Anisotropy =   110.7497
XX=   -27.0563   YX=    35.4312   ZX=    -1.0575
XY=    45.8820   YY=     2.9084   ZY=    32.2104
XZ=    -9.7952   YZ=    22.5539   ZZ=    85.7163
Eigenvalues:   -58.2961    25.5085    94.3559
  11  C    Isotropic =    27.8182   Anisotropy =   133.8515
XX=    16.8485   YX=   -11.2541   ZX=    10.5669
XY=    -5.2239   YY=   -27.0129   ZY=    59.4244
XZ=     4.3964   YZ=    56.3482   ZZ=    93.6190
Eigenvalues:   -51.8828    18.2848   117.0525
  12  C    Isotropic =    72.4871   Anisotropy =   119.5428
XX=    22.3685   YX=    31.2852   ZX=    -4.3691
XY=    44.5647   YY=    53.4893   ZY=    37.1174
XZ=    -5.4047   YZ=    26.0948   ZZ=   141.6034
Eigenvalues:    -6.3805    71.6594   152.1823
  13  C    Isotropic =    41.0275   Anisotropy =   194.5028
```

```
XX=   -44.4743   YX=   -13.9156   ZX=    20.3791
XY=   -16.4944   YY=    26.6236   ZY=    62.8626
XZ=    28.3384   YZ=    64.8653   ZZ=   140.9331
Eigenvalues:   -56.0911     8.4775   170.6960
  14  C    Isotropic =    80.2868   Anisotropy =   120.5515
XX=    74.7159   YX=     4.3288   ZX=     5.5714
XY=   -10.5408   YY=    26.3049   ZY=    56.7892
XZ=     3.4999   YZ=    48.6482   ZZ=   139.8396
Eigenvalues:     5.3026    74.9033   160.6545
  15  O    Isotropic =   206.6206   Anisotropy =    78.4849
XX=   154.9574   YX=     0.8563   ZX=    -0.6290
XY=    13.3799   YY=   207.8090   ZY=    20.8542
XZ=    27.8816   YZ=   -19.1512   ZZ=   257.0955
Eigenvalues:   152.3009   208.6171   258.9439
  16  O    Isotropic =   185.7369   Anisotropy =   117.2450
XX=   215.1326   YX=   -68.2205   ZX=    33.8876
XY=   -48.5267   YY=   158.4347   ZY=    30.3941
XZ=    32.5718   YZ=   -41.4141   ZZ=   183.6436
Eigenvalues:   118.9629   174.3476   263.9003
  17  O    Isotropic =   257.9565   Anisotropy =    37.2536
XX=   276.9986   YX=     1.4966   ZX=   -18.8869
XY=    -4.4206   YY=   250.4093   ZY=    -5.5752
XZ=    -9.7285   YZ=   -12.9464   ZZ=   246.4616
Eigenvalues:   235.2505   255.8268   282.7922
  18  C    Isotropic =   163.9280   Anisotropy =    41.0912
XX=   185.6671   YX=     8.6297   ZX=   -11.9259
XY=    11.5470   YY=   158.6915   ZY=    -9.6948
XZ=    -3.8909   YZ=    -5.9306   ZZ=   147.4255
Eigenvalues:   143.2526   157.2093   191.3221
  19  C    Isotropic =   167.4766   Anisotropy =    26.6892
XX=   166.7426   YX=     5.5783   ZX=    -9.6215
XY=     8.8688   YY=   170.0893   ZY=   -11.3767
XZ=    -8.6417   YZ=    -8.8934   ZZ=   165.5979
Eigenvalues:   156.0713   161.0891   185.2694
  20  C    Isotropic =    65.0145   Anisotropy =   117.3084
XX=   104.0677   YX=   -20.7698   ZX=    34.2601
XY=   -16.5351   YY=    -7.9446   ZY=    56.7643
XZ=    40.1766   YZ=    49.9464   ZZ=    98.9206
Eigenvalues:   -37.2684    89.0919   143.2202
  21  H    Isotropic =    30.0236   Anisotropy =     6.3580
XX=    27.3535   YX=    -0.2164   ZX=    -1.2075
XY=     0.4389   YY=    29.3250   ZY=    -1.6584
XZ=     0.0425   YZ=    -2.3483   ZZ=    33.3923
Eigenvalues:    27.2932    28.5154    34.2623
  22  H    Isotropic =    30.1284   Anisotropy =     9.0901
XX=    33.2345   YX=    -2.7438   ZX=     3.9831
XY=    -2.3703   YY=    29.9412   ZY=    -0.0815
XZ=     4.1456   YZ=    -0.2747   ZZ=    27.2096
Eigenvalues:    24.9428    29.2540    36.1885
  23  H    Isotropic =    30.4089   Anisotropy =    10.1689
XX=    29.3352   YX=     1.1362   ZX=     4.6913
XY=     1.1655   YY=    30.7410   ZY=     3.4986
```

```
XZ=     5.4384   YZ=     3.3591   ZZ=    31.1505
Eigenvalues:    24.7451    29.2935    37.1882
  24  H    Isotropic =    30.3296   Anisotropy =     6.3467
XX=    31.3385   YX=     1.5895   ZX=    -2.2500
XY=     1.2925   YY=    33.1133   ZY=    -1.7079
XZ=    -1.5671   YZ=    -1.2907   ZZ=    26.5370
Eigenvalues:    25.7411    30.6869    34.5607
  25  H    Isotropic =    29.6194   Anisotropy =     2.4315
XX=    29.9353   YX=    -1.6896   ZX=    -1.5958
XY=     0.5572   YY=    28.7097   ZY=     0.2148
XZ=     0.2604   YZ=     1.7091   ZZ=    30.2133
Eigenvalues:    28.2080    29.4098    31.2404
  26  H    Isotropic =    28.7916   Anisotropy =     4.2432
XX=    27.3202   YX=     0.7437   ZX=     0.7664
XY=    -1.2244   YY=    29.4858   ZY=    -2.0150
XZ=    -0.8311   YZ=    -2.1606   ZZ=    29.5687
Eigenvalues:    27.1734    27.5810    31.6203
  27  H    Isotropic =    27.6603   Anisotropy =     4.7751
XX=    26.6156   YX=     0.7957   ZX=    -0.9759
XY=    -0.7539   YY=    27.7269   ZY=     0.9954
XZ=    -2.9050   YZ=     3.0724   ZZ=    28.6383
Eigenvalues:    24.9162    27.2211    30.8437
  28  H    Isotropic =    30.2549   Anisotropy =     8.1778
XX=    29.4529   YX=     0.4793   ZX=    -2.3687
XY=     0.7078   YY=    32.7694   ZY=    -4.2320
XZ=    -2.2315   YZ=    -3.8645   ZZ=    28.5426
Eigenvalues:    25.3638    29.6942    35.7068
  29  H    Isotropic =    30.6075   Anisotropy =     9.5175
XX=    33.2849   YX=    -3.6415   ZX=     1.4875
XY=    -4.6778   YY=    31.7260   ZY=    -0.6918
XZ=     1.3915   YZ=    -0.4575   ZZ=    26.8117
Eigenvalues:    26.4733    28.3967    36.9525
  30  H    Isotropic =    30.4712   Anisotropy =     9.4376
XX=    27.6666   YX=    -0.3145   ZX=     0.5036
XY=    -0.1339   YY=    34.0856   ZY=     4.8458
XZ=     0.4200   YZ=     3.8744   ZZ=    29.6615
Eigenvalues:    26.7112    27.9395    36.7630
  31  H    Isotropic =    25.2315   Anisotropy =     6.8713
XX=    27.2644   YX=     2.4541   ZX=    -1.2333
XY=     2.3527   YY=    26.1115   ZY=    -2.0769
XZ=    -1.0075   YZ=    -2.1462   ZZ=    22.3185
Eigenvalues:    21.3764    24.5057    29.8123
  32  H    Isotropic =    25.3153   Anisotropy =     7.4536
XX=    30.1873   YX=     0.1289   ZX=    -0.7850
XY=     0.6078   YY=    24.0206   ZY=    -1.2092
XZ=    -0.6276   YZ=    -1.5733   ZZ=    21.7381
Eigenvalues:    21.0542    24.6074    30.2844
  33  H    Isotropic =    26.9913   Anisotropy =    18.3576
XX=    34.0850   YX=     4.1973   ZX=     7.0000
XY=     6.1018   YY=    28.0012   ZY=    -0.3502
XZ=     7.2408   YZ=     2.0585   ZZ=    18.8877
Eigenvalues:    15.9611    25.7831    39.2297
```

```
  34  H    Isotropic =    30.7097   Anisotropy =    15.0872
XX=    24.8069   YX=    -0.4457   ZX=    -3.8292
XY=    -0.2063   YY=    39.0388   ZY=    -4.1776
XZ=    -5.3409   YZ=    -4.7812   ZZ=    28.2835
Eigenvalues:    21.1672    30.1941    40.7679
  35  H    Isotropic =    29.6353   Anisotropy =     8.0410
XX=    33.2546   YX=    -3.1479   ZX=    -2.2043
XY=    -1.2694   YY=    30.1109   ZY=    -0.2902
XZ=    -3.1874   YZ=     0.0860   ZZ=    25.5403
Eigenvalues:    24.5777    29.3322    34.9959
  36  H    Isotropic =    29.3095   Anisotropy =     9.0928
XX=    31.1748   YX=     3.1075   ZX=     2.4320
XY=     3.5306   YY=    28.6783   ZY=     1.8339
XZ=     3.6383   YZ=     2.4756   ZZ=    28.0755
Eigenvalues:    26.1694    26.3878    35.3714
  37  H    Isotropic =    29.6902   Anisotropy =     7.7695
XX=    30.4090   YX=     2.1074   ZX=    -2.2219
XY=     0.0456   YY=    29.4115   ZY=    -4.4027
XZ=    -1.3926   YZ=    -4.8064   ZZ=    29.2501
Eigenvalues:    24.6715    29.5292    34.8698
  38  H    Isotropic =    29.8485   Anisotropy =     8.0225
XX=    33.5019   YX=     2.1474   ZX=     1.5922
XY=     2.9860   YY=    30.7018   ZY=    -0.9697
XZ=     2.1710   YZ=    -0.3818   ZZ=    25.3418
Eigenvalues:    24.6595    29.6891    35.1969
  39  H    Isotropic =    29.9295   Anisotropy =     4.7387
XX=    26.7597   YX=     0.2734   ZX=    -1.8001
XY=     1.0422   YY=    30.7295   ZY=    -1.2158
XZ=    -2.1152   YZ=     0.3247   ZZ=    32.2992
Eigenvalues:    26.0849    30.6148    33.0886
  40  H    Isotropic =    29.9227   Anisotropy =     8.3919
XX=    28.3104   YX=    -0.4337   ZX=    -0.9229
XY=    -1.6745   YY=    34.8743   ZY=    -1.6840
XZ=    -0.2589   YZ=    -2.6569   ZZ=    26.5834
Eigenvalues:    25.7722    28.4786    35.5173
  41  H    Isotropic =    26.5934   Anisotropy =     5.7181
XX=    27.8785   YX=    -3.1918   ZX=    -1.0575
XY=    -0.3780   YY=    26.4357   ZY=     1.6026
XZ=    -1.1838   YZ=     3.7525   ZZ=    25.4660
Eigenvalues:    23.2090    26.1658    30.4055
  42  H    Isotropic =    26.6391   Anisotropy =     7.1404
XX=    27.1702   YX=    -0.4145   ZX=    -1.3112
XY=    -2.5527   YY=    25.6202   ZY=     4.3022
XZ=    -0.5548   YZ=     4.2919   ZZ=    27.1270
Eigenvalues:    21.9524    26.5656    31.3994
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 52.20 | 74.52 | 92.18 | 98.08 | 126.83 | 155.44 |
| intensities | 0.21 | 1.49 | 0.14 | 0.76 | 5.74 | 0.71 |
| reduc. mass | 1.21 | 0.86 | 1.07 | 1.16 | 0.24 | 0.60 |
| force const | 0.00 | 0.00 | 0.01 | 0.01 | 0.00 | 0.01 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 171.61 | 200.65 | 219.31 | 237.34 | 249.02 | 255.54 |
| intensities | 0.89 | 2.67 | 0.76 | 0.26 | 10.13 | 2.88 |
| reduc. mass | 1.11 | 0.77 | 1.16 | 0.64 | 1.13 | 1.37 |
| force const | 0.02 | 0.02 | 0.03 | 0.02 | 0.04 | 0.05 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 271.90 | 280.74 | 303.90 | 318.21 | 329.60 | 331.83 |
| intensities | 2.62 | 0.33 | 2.45 | 1.52 | 1.10 | 1.56 |
| reduc. mass | 0.73 | 0.23 | 2.26 | 0.39 | 1.44 | 0.25 |
| force const | 0.03 | 0.01 | 0.12 | 0.02 | 0.09 | 0.02 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 362.04 | 424.78 | 433.82 | 444.54 | 480.01 | 491.50 |
| intensities | 1.73 | 11.92 | 6.59 | 16.79 | 7.22 | 3.02 |
| reduc. mass | 0.55 | 0.61 | 0.34 | 0.85 | 0.60 | 1.15 |
| force const | 0.04 | 0.07 | 0.04 | 0.10 | 0.08 | 0.16 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 521.04 | 524.85 | 537.26 | 545.25 | 566.74 | 606.24 |
| intensities | 2.89 | 10.20 | 1.38 | 3.07 | 32.72 | 21.51 |
| reduc. mass | 0.53 | 1.64 | 0.75 | 0.64 | 0.51 | 2.03 |
| force const | 0.09 | 0.27 | 0.13 | 0.11 | 0.10 | 0.44 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 633.33 | 667.43 | 684.24 | 713.86 | 714.97 | 736.06 |
| intensities | 88.59 | 9.35 | 4.89 | 2.96 | 15.71 | 1.44 |
| reduc. mass | 0.66 | 0.83 | 1.24 | 1.04 | 0.46 | 0.55 |
| force const | 0.16 | 0.22 | 0.34 | 0.31 | 0.14 | 0.18 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 748.38 | 798.56 | 810.69 | 834.26 | 869.61 | 926.08 |
| intensities | 4.52 | 4.32 | 4.13 | 2.15 | 10.32 | 4.96 |
| reduc. mass | 1.46 | 0.51 | 0.91 | 2.73 | 0.58 | 0.73 |
| force const | 0.48 | 0.19 | 0.35 | 1.12 | 0.26 | 0.37 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 928.84 | 937.68 | 964.15 | 1006.26 | 1012.77 | 1016.92 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 4.80 | 11.76 | 6.28 | 6.11 | 7.18 | 2.68 |
| reduc. mass | 0.66 | 1.50 | 0.30 | 0.29 | 0.29 | 0.32 |
| force const | 0.34 | 0.78 | 0.16 | 0.18 | 0.17 | 0.20 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1032.07 | 1047.06 | 1057.36 | 1059.76 | 1068.80 | 1093.03 |
| intensities | 15.84 | 22.38 | 7.06 | 6.67 | 21.83 | 19.42 |
| reduc. mass | 0.39 | 0.32 | 0.35 | 0.31 | 0.29 | 0.60 |
| force const | 0.24 | 0.21 | 0.23 | 0.21 | 0.19 | 0.42 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1103.34 | 1115.84 | 1128.89 | 1153.73 | 1170.69 | 1223.43 |
| intensities | 60.14 | 32.98 | 22.25 | 47.17 | 23.54 | 21.45 |
| reduc. mass | 0.64 | 0.36 | 0.43 | 0.92 | 0.56 | 0.32 |
| force const | 0.46 | 0.27 | 0.32 | 0.72 | 0.45 | 0.28 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1227.09 | 1253.14 | 1255.40 | 1282.18 | 1315.40 | 1330.93 |
| intensities | 31.61 | 106.28 | 11.94 | 49.90 | 106.91 | 21.82 |
| reduc. mass | 0.56 | 0.91 | 0.25 | 0.98 | 0.27 | 0.61 |
| force const | 0.49 | 0.84 | 0.23 | 0.95 | 0.27 | 0.63 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1341.65 | 1387.42 | 1397.76 | 1409.27 | 1414.80 | 1473.20 |
| intensities | 77.48 | 102.56 | 86.64 | 201.81 | 286.83 | 14.12 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.79 | 0.61 | 0.96 | 0.37 | 0.58 | 1.42 |
| force const | 0.83 | 0.69 | 1.10 | 0.43 | 0.69 | 1.81 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1488.34 | 1497.22 | 1510.76 | 1522.43 | 1534.46 | 1539.04 |
| intensities | 10.22 | 5.22 | 156.19 | 25.14 | 69.66 | 6.48 |
| reduc. mass | 0.72 | 0.83 | 1.26 | 1.91 | 0.60 | 0.47 |
| force const | 0.94 | 1.10 | 1.69 | 2.61 | 0.83 | 0.66 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1569.21 | 1577.68 | 1591.45 | 1627.25 | 1636.54 | 1646.76 |
| intensities | 46.96 | 28.73 | 33.69 | 9.67 | 81.98 | 93.60 |
| reduc. mass | 0.54 | 0.54 | 0.39 | 0.42 | 0.23 | 0.34 |
| force const | 0.78 | 0.79 | 0.58 | 0.65 | 0.36 | 0.54 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1651.94 | 1655.05 | 1659.30 | 1659.90 | 1662.60 | 1662.93 |
| intensities | 16.88 | 32.36 | 8.45 | 21.99 | 20.91 | 21.60 |
| reduc. mass | 0.58 | 0.23 | 0.24 | 0.29 | 0.36 | 0.23 |
| force const | 0.94 | 0.37 | 0.39 | 0.46 | 0.59 | 0.38 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1677.25 | 1679.80 | 1684.74 | 1687.04 | 1728.44 | 1798.34 |
| intensities | 4.15 | 26.01 | 5.26 | 137.31 | 32.60 | 738.62 |
| reduc. mass | 0.34 | 0.24 | 0.28 | 0.79 | 1.06 | 1.56 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 0.56 | 0.40 | 0.47 | 1.33 | 1.87 | 2.97 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1831.30 | 1891.41 | 3023.27 | 3028.03 | 3033.54 | 3051.15 |
| intensities | 392.93 | 11.79 | 405.72 | 624.97 | 370.87 | 493.84 |
| reduc. mass | 1.37 | 0.87 | 0.31 | 0.16 | 0.15 | 0.45 |
| force const | 2.71 | 1.84 | 1.68 | 0.89 | 0.81 | 2.48 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3060.39 | 3074.22 | 3082.44 | 3089.45 | 3092.82 | 3120.06 |
| intensities | 452.84 | 363.73 | 220.85 | 108.50 | 409.94 | 206.64 |
| reduc. mass | 0.41 | 0.88 | 0.56 | 0.54 | 0.46 | 0.39 |
| force const | 2.25 | 4.91 | 3.14 | 3.05 | 2.59 | 2.24 |

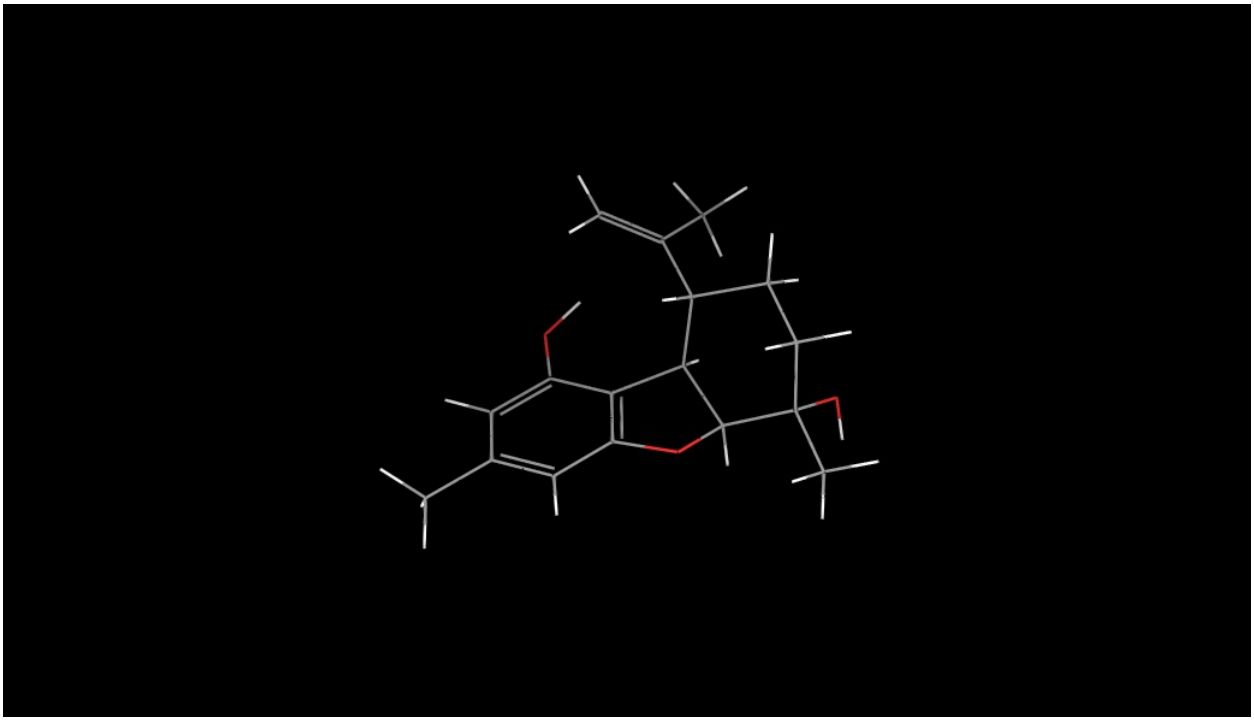
| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3124.12 | 3132.33 | 3134.93 | 3143.39 | 3145.37 | 3146.46 |
| intensities | 732.16 | 352.14 | 470.68 | 482.73 | 388.19 | 91.11 |
| reduc. mass | 0.36 | 0.42 | 0.47 | 0.44 | 0.40 | 0.41 |
| force const | 2.09 | 2.44 | 2.70 | 2.54 | 2.36 | 2.40 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3152.39 | 3156.40 | 3172.19 | 3196.95 | 3839.06 | 3866.28 |
| intensities | 395.61 | 307.86 | 436.17 | 267.52 | 50.47 | 76.02 |
| reduc. mass | 0.71 | 0.37 | 0.58 | 0.55 | 0.94 | 0.94 |
| force const | 4.16 | 2.18 | 3.46 | 3.33 | 8.20 | 8.32 |

Number of imaginary frequencies: 0

Conformation 4

Boltzmann Population = 19.2% (relative energy = 0.46 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.980672 hartrees

Total enthalpy, Htot (Utot + pV): -885.979728 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.042557 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.019200 | -0.576900 | -2.688800 |
| 2 | 6 | 0 | -4.552000 | -0.288400 | -2.995700 |
| 3 | 6 | 0 | -3.842700 | -1.568500 | -3.454100 |
| 4 | 6 | 0 | -3.950000 | -2.700900 | -2.394600 |
| 5 | 6 | 0 | -5.370500 | -2.847400 | -1.805900 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 6 | 0 | -6.146000 | -1.558700 | -1.527600 |
| 7 | 6 | 0 | -7.603200 | -1.868400 | -1.207500 |
| 8 | 6 | 0 | -2.392600 | -1.335000 | -3.824900 |
| 9 | 6 | 0 | -3.837800 | -4.065900 | -3.046100 |
| 10 | 6 | 0 | -5.136600 | -4.533600 | -3.253300 |
| 11 | 6 | 0 | -2.775300 | -4.835800 | -3.504500 |
| 12 | 6 | 0 | -3.043600 | -6.056000 | -4.138000 |
| 13 | 6 | 0 | -4.349300 | -6.498500 | -4.334800 |
| 14 | 6 | 0 | -5.429600 | -5.723300 | -3.890100 |
| 15 | 8 | 0 | -1.472600 | -4.479600 | -3.346800 |
| 16 | 8 | 0 | -6.078100 | -3.681400 | -2.737600 |
| 17 | 8 | 0 | -5.511900 | -0.923400 | -0.419000 |
| 18 | 6 | 0 | -4.611500 | -7.827900 | -4.997400 |
| 19 | 6 | 0 | -1.555800 | -0.519900 | -2.870700 |
| 20 | 6 | 0 | -1.878600 | -1.844600 | -4.948300 |
| 21 | 1 | 0 | -6.515800 | -1.007300 | -3.566600 |
| 22 | 1 | 0 | -6.549400 | 0.341300 | -2.416800 |
| 23 | 1 | 0 | -4.466900 | 0.469900 | -3.781800 |
| 24 | 1 | 0 | -4.077600 | 0.114300 | -2.094700 |
| 25 | 1 | 0 | -4.364200 | -1.931000 | -4.349700 |
| 26 | 1 | 0 | -3.231500 | -2.531900 | -1.585300 |
| 27 | 1 | 0 | -5.294300 | -3.410900 | -0.860000 |
| 28 | 1 | 0 | -8.122100 | -0.945000 | -0.937600 |
| 29 | 1 | 0 | -8.099400 | -2.329600 | -2.063400 |
| 30 | 1 | 0 | -7.672100 | -2.567600 | -0.365600 |
| 31 | 1 | 0 | -2.199900 | -6.644800 | -4.482600 |
| 32 | 1 | 0 | -6.456200 | -6.047000 | -4.021500 |
| 33 | 1 | 0 | -1.425000 | -3.514400 | -3.303200 |
| 34 | 1 | 0 | -5.688600 | -1.452600 | 0.368200 |
| 35 | 1 | 0 | -3.757000 | -8.147500 | -5.597400 |
| 36 | 1 | 0 | -4.802200 | -8.603200 | -4.248100 |
| 37 | 1 | 0 | -5.488900 | -7.777300 | -5.647400 |
| 38 | 1 | 0 | -0.498400 | -0.558800 | -3.140900 |
| 39 | 1 | 0 | -1.871100 | 0.528600 | -2.880100 |
| 40 | 1 | 0 | -1.663300 | -0.869200 | -1.837500 |
| 41 | 1 | 0 | -0.834700 | -1.701300 | -5.213400 |
| 42 | 1 | 0 | -2.489400 | -2.424100 | -5.634800 |

---

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 152.3848 Anisotropy = 19.8564

XX= 145.8604 YX= 0.5803 ZX= 2.3797

XY= -4.6647 YY= 160.2744 ZY= 7.8815

XZ= -3.2012 YZ= 9.3508 ZZ= 151.0195

Eigenvalues: 145.0664 146.4655 165.6224

2 C Isotropic = 161.1949 Anisotropy = 14.8822

XX= 164.7129 YX= -5.2878 ZX= 6.9486

XY= -4.0307 YY= 163.4494 ZY= 0.1742

XZ= 8.0999 YZ= -0.0523 ZZ= 155.4225

```
Eigenvalues:   150.7670   161.7014   171.1164
   3  C    Isotropic =   133.6351   Anisotropy =    14.5021
XX=   135.9300   YX=    -1.4353   ZX=     2.2125
XY=     6.1692   YY=   138.7770   ZY=    -6.7507
XZ=     0.3789   YZ=   -10.0267   ZZ=   126.1983
Eigenvalues:   121.6559   135.9463   143.3032
   4  C    Isotropic =   141.6103   Anisotropy =    19.5890
XX=   147.8333   YX=    -0.6747   ZX=     1.8607
XY=     0.6048   YY=   148.2770   ZY=     0.9924
XZ=     6.6297   YZ=    23.4665   ZZ=   128.7208
Eigenvalues:   122.2617   147.8997   154.6697
   5  C    Isotropic =    94.0520   Anisotropy =    57.1193
XX=   117.9421   YX=     8.5270   ZX=   -23.8901
XY=    -1.5511   YY=    85.8668   ZY=   -18.2042
XZ=   -26.5092   YZ=    -9.9077   ZZ=    78.3472
Eigenvalues:    60.8910    89.1336   132.1316
   6  C    Isotropic =   116.4166   Anisotropy =    53.5649
XX=   120.0185   YX=    10.0741   ZX=   -27.0665
XY=     7.5012   YY=   108.2799   ZY=   -11.6657
XZ=   -25.3344   YZ=   -14.2883   ZZ=   120.9516
Eigenvalues:    93.5059   103.6174   152.1266
   7  C    Isotropic =   157.4143   Anisotropy =    45.5850
XX=   140.6445   YX=    -7.7918   ZX=     0.0343
XY=    -4.1282   YY=   186.9140   ZY=    -2.6842
XZ=    -0.2042   YZ=    -2.1992   ZZ=   144.6844
Eigenvalues:   139.8566   144.5820   187.8043
   8  C    Isotropic =    27.5435   Anisotropy =   193.8710
XX=    60.9597   YX=    -8.2142   ZX=    79.4739
XY=   -15.1757   YY=   -51.1750   ZY=    66.5810
XZ=    82.0523   YZ=    67.6733   ZZ=    72.8459
Eigenvalues:   -94.6963    20.5361   156.7909
   9  C    Isotropic =    66.6266   Anisotropy =   112.4407
XX=    19.6435   YX=     2.5725   ZX=     9.3383
XY=   -12.7100   YY=    59.3641   ZY=    37.1795
XZ=    22.2777   YZ=    42.3856   ZZ=   120.8724
Eigenvalues:    13.4840    44.8088   141.5871
  10  C    Isotropic =    20.6233   Anisotropy =   109.6389
XX=   -26.4034   YX=    36.5012   ZX=    -0.9288
XY=    46.9373   YY=     2.4386   ZY=    30.5838
XZ=    -9.5518   YZ=    21.5381   ZZ=    85.8347
Eigenvalues:   -58.7902    26.9442    93.7159
  11  C    Isotropic =    27.5446   Anisotropy =   134.3470
XX=    15.8462   YX=   -11.8181   ZX=    10.8569
XY=    -6.2324   YY=   -28.0563   ZY=    58.1134
XZ=     5.3495   YZ=    55.0567   ZZ=    94.8438
Eigenvalues:   -52.0424    17.5669   117.1093
  12  C    Isotropic =    72.1812   Anisotropy =   117.5898
XX=    23.3311   YX=    32.8893   ZX=    -4.4604
XY=    45.0064   YY=    52.3920   ZY=    35.4381
XZ=    -4.3017   YZ=    24.8070   ZZ=   140.8204
Eigenvalues:    -6.7522    72.7214   150.5744
  13  C    Isotropic =    41.4940   Anisotropy =   193.8040
```

```
XX=   -44.1851   YX=   -13.8042   ZX=    20.6092
XY=   -16.6704   YY=    26.0068   ZY=    61.0018
XZ=    28.2230   YZ=    62.9244   ZZ=   142.6604
Eigenvalues:   -55.5950     9.3804   170.6967
  14  C    Isotropic =    80.7343   Anisotropy =   121.6919
XX=    74.4997   YX=     4.1102   ZX=     5.9979
XY=   -11.3247   YY=    25.5492   ZY=    55.5907
XZ=     4.5810   YZ=    47.6074   ZZ=   142.1538
Eigenvalues:     5.5950    74.7456   161.8622
  15  O    Isotropic =   205.5088   Anisotropy =    79.9187
XX=   153.0886   YX=     1.4577   ZX=    -0.7765
XY=    13.4748   YY=   206.5544   ZY=    21.2381
XZ=    28.6754   YZ=   -19.5835   ZZ=   256.8834
Eigenvalues:   150.3004   207.4381   258.7879
  16  O    Isotropic =   184.6663   Anisotropy =   112.6464
XX=   211.9105   YX=   -66.6260   ZX=    31.8326
XY=   -46.9588   YY=   157.2183   ZY=    29.4496
XZ=    31.5013   YZ=   -41.3627   ZZ=   184.8702
Eigenvalues:   119.1577   175.0774   259.7640
  17  O    Isotropic =   245.8725   Anisotropy =    64.3757
XX=   227.4565   YX=     9.5526   ZX=    -3.8651
XY=    11.6551   YY=   225.8607   ZY=    18.9320
XZ=   -19.4561   YZ=     8.6666   ZZ=   284.3001
Eigenvalues:   211.5465   237.2813   288.7896
  18  C    Isotropic =   163.9719   Anisotropy =    41.1169
XX=   186.7583   YX=     6.7674   ZX=   -10.6649
XY=    11.6816   YY=   157.9768   ZY=    -8.9597
XZ=    -4.1787   YZ=    -5.4624   ZZ=   147.1806
Eigenvalues:   143.3964   157.1362   191.3832
  19  C    Isotropic =   167.3358   Anisotropy =    26.9759
XX=   166.7634   YX=     5.4662   ZX=    -9.9308
XY=     8.6748   YY=   169.5252   ZY=   -11.6307
XZ=    -8.7313   YZ=    -9.2092   ZZ=   165.7187
Eigenvalues:   155.7096   160.9780   185.3197
  20  C    Isotropic =    66.3044   Anisotropy =   115.0753
XX=   105.7215   YX=   -21.6705   ZX=    34.2705
XY=   -17.4200   YY=    -4.1907   ZY=    57.4724
XZ=    39.7991   YZ=    51.0406   ZZ=    97.3825
Eigenvalues:   -35.5190    91.4110   143.0213
  21  H    Isotropic =    30.1641   Anisotropy =     6.3247
XX=    27.6264   YX=    -0.2627   ZX=    -1.1930
XY=     0.5833   YY=    29.4411   ZY=    -1.9290
XZ=     0.1081   YZ=    -2.2893   ZZ=    33.4247
Eigenvalues:    27.5750    28.5367    34.3805
  22  H    Isotropic =    30.0538   Anisotropy =     9.0349
XX=    33.1489   YX=    -2.6668   ZX=     3.9668
XY=    -2.4187   YY=    29.7591   ZY=    -0.0311
XZ=     4.1123   YZ=    -0.2639   ZZ=    27.2533
Eigenvalues:    24.9566    29.1277    36.0771
  23  H    Isotropic =    30.6234   Anisotropy =    10.0343
XX=    29.6998   YX=     1.1151   ZX=     4.6790
XY=     1.2237   YY=    31.2352   ZY=     3.5844
```

```
XZ=     5.4880   YZ=     3.2436   ZZ=    30.9352
Eigenvalues:    24.8365    29.7208    37.3129
  24  H    Isotropic =    29.6088   Anisotropy =     6.0288
XX=    30.2345   YX=     1.2562   ZX=    -2.6697
XY=     1.0162   YY=    32.3528   ZY=    -1.5675
XZ=    -2.0746   YZ=    -1.3728   ZZ=    26.2390
Eigenvalues:    25.0297    30.1686    33.6280
  25  H    Isotropic =    29.6178   Anisotropy =     2.5137
XX=    29.8844   YX=    -1.7320   ZX=    -1.4498
XY=     0.3618   YY=    28.7652   ZY=     0.3148
XZ=     0.3055   YZ=     1.8730   ZZ=    30.2038
Eigenvalues:    28.1032    29.4565    31.2936
  26  H    Isotropic =    28.4948   Anisotropy =     4.2942
XX=    26.8472   YX=     0.8322   ZX=     0.5171
XY=    -1.1658   YY=    29.3318   ZY=    -1.9666
XZ=    -0.9093   YZ=    -2.1111   ZZ=    29.3055
Eigenvalues:    26.7277    27.3991    31.3576
  27  H    Isotropic =    27.9528   Anisotropy =     4.8159
XX=    26.9462   YX=     0.7631   ZX=    -1.1700
XY=    -0.6404   YY=    28.0307   ZY=     0.9144
XZ=    -3.1686   YZ=     2.9707   ZZ=    28.8815
Eigenvalues:    25.0463    27.6487    31.1634
  28  H    Isotropic =    30.5405   Anisotropy =     9.1048
XX=    32.8196   YX=    -3.4016   ZX=     1.4953
XY=    -4.7282   YY=    31.7311   ZY=    -0.6189
XZ=     1.5757   YZ=    -0.3971   ZZ=    27.0708
Eigenvalues:    26.5937    28.4174    36.6104
  29  H    Isotropic =    29.9476   Anisotropy =     8.4542
XX=    29.0352   YX=     0.4715   ZX=    -2.2881
XY=     0.9670   YY=    32.6565   ZY=    -4.4169
XZ=    -2.2151   YZ=    -3.7983   ZZ=    28.1510
Eigenvalues:    25.0477    29.2113    35.5837
  30  H    Isotropic =    30.8590   Anisotropy =     8.9699
XX=    28.3715   YX=    -0.2809   ZX=     0.3030
XY=    -0.1296   YY=    34.5500   ZY=     4.6483
XZ=     0.2689   YZ=     3.4611   ZZ=    29.6554
Eigenvalues:    27.2569    28.4812    36.8389
  31  H    Isotropic =    25.2416   Anisotropy =     6.7818
XX=    27.2914   YX=     2.3833   ZX=    -1.1897
XY=     2.3548   YY=    26.1165   ZY=    -2.0088
XZ=    -0.9741   YZ=    -2.1103   ZZ=    22.3168
Eigenvalues:    21.4143    24.5476    29.7628
  32  H    Isotropic =    25.3327   Anisotropy =     7.4956
XX=    30.2441   YX=     0.0223   ZX=    -0.7623
XY=     0.5955   YY=    24.0268   ZY=    -1.1610
XZ=    -0.6408   YZ=    -1.4761   ZZ=    21.7271
Eigenvalues:    21.0987    24.5697    30.3298
  33  H    Isotropic =    26.7861   Anisotropy =    18.7803
XX=    34.0867   YX=     4.2124   ZX=     7.1465
XY=     6.1420   YY=    27.7104   ZY=    -0.1842
XZ=     7.4216   YZ=     2.2695   ZZ=    18.5612
Eigenvalues:    15.5982    25.4539    39.3063
```

```
  34  H    Isotropic =    31.8333   Anisotropy =    16.5043
XX=    27.0674   YX=     0.9178   ZX=    -3.9035
XY=     0.1311   YY=    28.9936   ZY=     5.6189
XZ=    -3.3350   YZ=     6.5354   ZZ=    39.4390
Eigenvalues:    24.3774    28.2864    42.8362
  35  H    Isotropic =    29.7427   Anisotropy =     7.9523
XX=    33.6859   YX=    -3.3490   ZX=    -1.4946
XY=    -1.1808   YY=    30.2586   ZY=    -0.7619
XZ=    -2.3954   YZ=    -0.4178   ZZ=    25.2837
Eigenvalues:    24.6364    29.5476    35.0443
  36  H    Isotropic =    29.3280   Anisotropy =     9.0307
XX=    30.9851   YX=     3.3040   ZX=     1.9984
XY=     3.3717   YY=    29.4480   ZY=     2.1691
XZ=     3.2234   YZ=     2.9731   ZZ=    27.5510
Eigenvalues:    25.7318    26.9038    35.3485
  37  H    Isotropic =    29.5860   Anisotropy =     7.9093
XX=    30.2771   YX=     1.9430   ZX=    -2.4128
XY=     0.1042   YY=    28.4684   ZY=    -4.1490
XZ=    -1.7933   YZ=    -4.6917   ZZ=    30.0127
Eigenvalues:    24.6886    29.2106    34.8589
  38  H    Isotropic =    29.9872   Anisotropy =     8.3352
XX=    28.3488   YX=    -0.3708   ZX=    -0.9436
XY=    -1.6275   YY=    34.8541   ZY=    -1.7584
XZ=    -0.2722   YZ=    -2.7986   ZZ=    26.7588
Eigenvalues:    25.8681    28.5496    35.5440
  39  H    Isotropic =    29.8427   Anisotropy =     7.9920
XX=    33.6057   YX=     2.1155   ZX=     1.5239
XY=     2.8894   YY=    30.6052   ZY=    -1.0991
XZ=     2.1004   YZ=    -0.5122   ZZ=    25.3174
Eigenvalues:    24.6264    29.7311    35.1707
  40  H    Isotropic =    29.7903   Anisotropy =     4.6031
XX=    26.5717   YX=     0.3068   ZX=    -1.7926
XY=     0.9965   YY=    30.6540   ZY=    -1.0742
XZ=    -2.0640   YZ=     0.4510   ZZ=    32.1453
Eigenvalues:    25.9101    30.6018    32.8591
  41  H    Isotropic =    26.6361   Anisotropy =     5.7531
XX=    27.8035   YX=    -3.2125   ZX=    -1.0123
XY=    -0.4107   YY=    26.6244   ZY=     1.5996
XZ=    -1.1616   YZ=     3.8246   ZZ=    25.4805
Eigenvalues:    23.2573    26.1796    30.4716
  42  H    Isotropic =    26.6493   Anisotropy =     7.0819
XX=    27.1200   YX=    -0.4065   ZX=    -1.2634
XY=    -2.5796   YY=    25.7207   ZY=     4.3340
XZ=    -0.4795   YZ=     4.2050   ZZ=    27.1071
Eigenvalues:    22.0201    26.5572    31.3706
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 42.13 | 70.77 | 89.60 | 94.75 | 105.47 | 155.90 |
| intensities | 0.99 | 1.81 | 0.83 | 0.03 | 0.41 | 0.67 |
| reduc. mass | 0.62 | 0.70 | 0.46 | 1.18 | 2.23 | 1.38 |
| force const | 0.00 | 0.00 | 0.00 | 0.01 | 0.01 | 0.02 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 169.47 | 195.72 | 229.79 | 238.56 | 245.31 | 260.12 |
| intensities | 1.02 | 1.86 | 2.34 | 1.90 | 6.05 | 0.59 |
| reduc. mass | 0.68 | 0.73 | 1.06 | 0.61 | 0.75 | 1.27 |
| force const | 0.01 | 0.02 | 0.03 | 0.02 | 0.03 | 0.05 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 271.47 | 274.18 | 303.52 | 309.76 | 314.64 | 342.16 |
| intensities | 1.56 | 1.03 | 1.93 | 5.59 | 3.25 | 1.08 |
| reduc. mass | 0.66 | 0.78 | 2.36 | 0.40 | 0.34 | 1.36 |
| force const | 0.03 | 0.03 | 0.13 | 0.02 | 0.02 | 0.09 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 356.44 | 403.83 | 430.77 | 434.68 | 473.79 | 491.49 |
| intensities | 1.26 | 4.13 | 43.03 | 7.12 | 7.00 | 13.47 |
| reduc. mass | 0.67 | 0.96 | 0.50 | 0.68 | 0.48 | 1.01 |
| force const | 0.05 | 0.09 | 0.06 | 0.08 | 0.06 | 0.14 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 510.08 | 525.25 | 541.52 | 561.49 | 568.37 | 601.12 |
| intensities | 9.17 | 7.68 | 6.22 | 10.50 | 31.73 | 23.62 |
| reduc. mass | 0.65 | 1.50 | 0.73 | 0.66 | 0.51 | 2.21 |
| force const | 0.10 | 0.24 | 0.13 | 0.12 | 0.10 | 0.47 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 646.90 | 670.43 | 683.43 | 711.95 | 723.87 | 749.36 |
| intensities | 110.22 | 1.10 | 2.68 | 2.37 | 25.09 | 2.48 |
| reduc. mass | 0.67 | 1.04 | 1.04 | 1.03 | 0.40 | 1.61 |
| force const | 0.16 | 0.27 | 0.29 | 0.31 | 0.12 | 0.53 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 761.55 | 805.40 | 830.70 | 837.08 | 870.31 | 923.88 |
| intensities | 3.53 | 4.86 | 9.63 | 5.55 | 13.51 | 2.75 |
| reduc. mass | 0.62 | 0.55 | 0.79 | 1.73 | 0.56 | 0.78 |
| force const | 0.21 | 0.21 | 0.32 | 0.71 | 0.25 | 0.39 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 928.31 | 966.77 | 977.76 | 1006.20 | 1013.05 | 1019.23 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 7.80 | 8.02 | 17.82 | 15.09 | 1.50 | 2.31 |
| reduc. mass | 0.65 | 0.28 | 1.04 | 0.36 | 0.24 | 0.36 |
| force const | 0.33 | 0.15 | 0.58 | 0.21 | 0.15 | 0.22 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1030.12 | 1045.52 | 1055.33 | 1060.70 | 1072.50 | 1094.81 |
| intensities | 17.25 | 20.47 | 11.74 | 14.39 | 17.53 | 29.48 |
| reduc. mass | 0.50 | 0.37 | 0.51 | 0.20 | 0.31 | 0.64 |
| force const | 0.31 | 0.24 | 0.33 | 0.13 | 0.21 | 0.45 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1109.69 | 1125.99 | 1138.14 | 1170.13 | 1184.77 | 1213.29 |
| intensities | 55.80 | 27.28 | 6.49 | 38.35 | 11.34 | 75.16 |
| reduc. mass | 0.39 | 0.41 | 0.46 | 0.59 | 1.18 | 0.58 |
| force const | 0.28 | 0.31 | 0.35 | 0.48 | 0.98 | 0.50 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1244.58 | 1247.19 | 1263.24 | 1281.03 | 1322.43 | 1344.50 |
| intensities | 97.51 | 37.59 | 49.86 | 13.55 | 31.94 | 115.04 |
| reduc. mass | 0.63 | 0.23 | 0.38 | 0.20 | 0.30 | 0.62 |
| force const | 0.58 | 0.21 | 0.36 | 0.20 | 0.31 | 0.66 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1353.40 | 1392.06 | 1398.93 | 1409.44 | 1414.24 | 1479.04 |
| intensities | 47.75 | 115.54 | 136.02 | 193.94 | 265.34 | 5.94 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 1.17 | 0.63 | 0.77 | 0.48 | 0.35 | 1.51 |
| force const | 1.26 | 0.72 | 0.89 | 0.57 | 0.42 | 1.94 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1484.90 | 1490.32 | 1512.48 | 1521.09 | 1538.50 | 1546.72 |
| intensities | 5.43 | 28.43 | 179.54 | 9.96 | 60.37 | 14.20 |
| reduc. mass | 0.81 | 0.63 | 1.47 | 2.46 | 0.57 | 0.75 |
| force const | 1.05 | 0.82 | 1.98 | 3.35 | 0.79 | 1.06 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1568.23 | 1582.25 | 1605.88 | 1631.64 | 1641.69 | 1649.44 |
| intensities | 58.27 | 51.76 | 27.07 | 23.82 | 53.20 | 44.94 |
| reduc. mass | 0.60 | 0.58 | 0.66 | 0.38 | 0.21 | 0.29 |
| force const | 0.86 | 0.85 | 1.01 | 0.60 | 0.34 | 0.47 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1654.54 | 1658.91 | 1660.73 | 1663.82 | 1667.19 | 1671.84 |
| intensities | 28.79 | 20.09 | 19.48 | 26.74 | 31.57 | 24.88 |
| reduc. mass | 0.28 | 0.33 | 0.21 | 0.14 | 0.15 | 0.16 |
| force const | 0.45 | 0.54 | 0.35 | 0.22 | 0.24 | 0.26 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1675.21 | 1683.08 | 1688.98 | 1731.71 | 1750.10 | 1811.89 |
| intensities | 14.39 | 88.62 | 21.36 | 35.82 | 200.41 | 626.09 |
| reduc. mass | 0.34 | 0.59 | 0.30 | 1.05 | 1.64 | 1.70 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 0.56 | 0.99 | 0.50 | 1.85 | 2.96 | 3.29 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1885.05 | 1905.62 | 3024.77 | 3025.80 | 3043.36 | 3057.59 |
| intensities | 171.39 | 230.96 | 281.60 | 597.76 | 843.81 | 418.98 |
| reduc. mass | 0.53 | 0.81 | 0.14 | 0.14 | 0.16 | 0.14 |
| force const | 1.11 | 1.74 | 0.77 | 0.74 | 0.87 | 0.79 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3060.38 | 3066.82 | 3086.13 | 3103.19 | 3120.27 | 3129.05 |
| intensities | 589.76 | 514.12 | 225.63 | 162.19 | 224.09 | 91.67 |
| reduc. mass | 0.28 | 0.26 | 0.48 | 0.46 | 0.27 | 0.12 |
| force const | 1.55 | 1.42 | 2.72 | 2.62 | 1.55 | 0.68 |

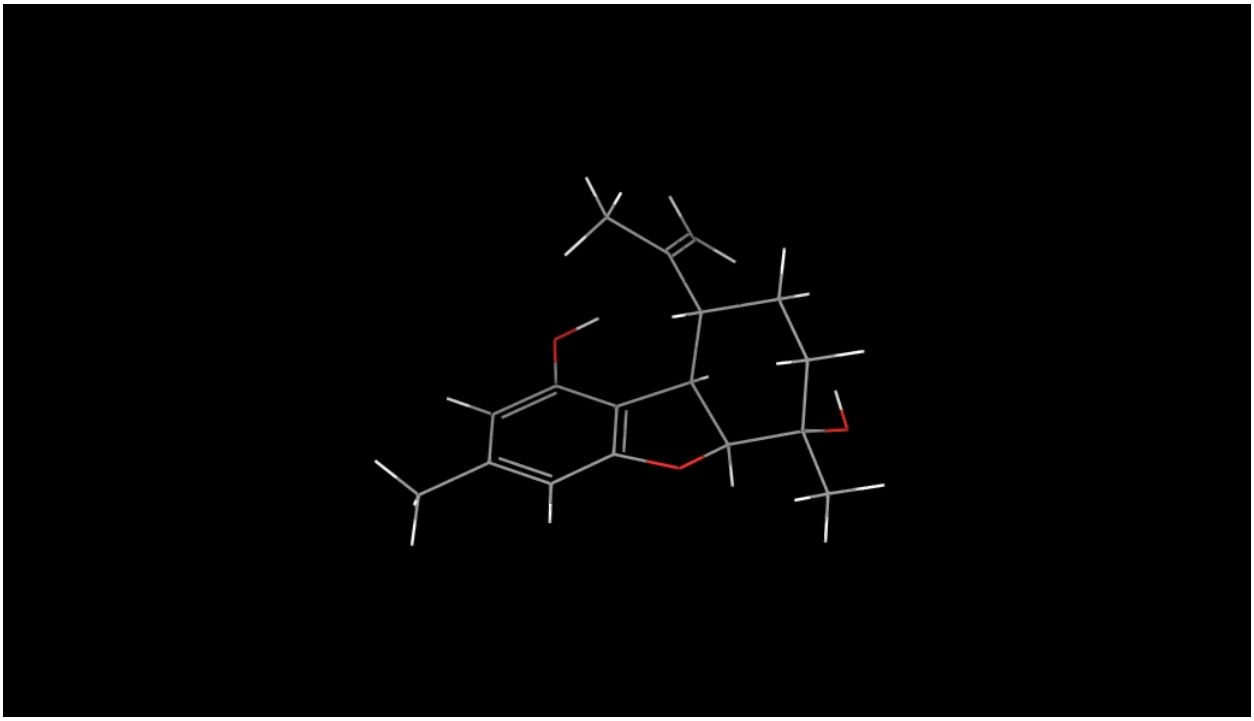
| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3131.79 | 3134.63 | 3136.99 | 3142.57 | 3147.79 | 3148.73 |
| intensities | 155.38 | 360.82 | 566.58 | 404.96 | 225.90 | 62.28 |
| reduc. mass | 0.13 | 0.28 | 0.44 | 0.13 | 0.17 | 0.23 |
| force const | 0.74 | 1.65 | 2.56 | 0.78 | 1.00 | 1.33 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3158.85 | 3163.83 | 3194.68 | 3232.30 | 3838.50 | 3856.86 |
| intensities | 196.03 | 890.69 | 475.07 | 460.89 | 91.88 | 69.57 |
| reduc. mass | 0.37 | 0.15 | 0.48 | 0.15 | 0.89 | 0.89 |
| force const | 2.15 | 0.86 | 2.87 | 0.91 | 7.73 | 7.80 |

Number of imaginary frequencies: 0

Conformation 5

Boltzmann Population = 4.0% (relative energy = 1.39 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.980886 hartrees

Total enthalpy, Htot (Utot + pV): -885.979942 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.042752 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.131500 | -0.632700 | -2.559300 |
| 2 | 6 | 0 | -4.661300 | -0.329500 | -2.856400 |
| 3 | 6 | 0 | -3.952600 | -1.603700 | -3.330400 |
| 4 | 6 | 0 | -4.050500 | -2.739700 | -2.281700 |

| | | | | | |
|---|---|---|---|---|---|
| 5 | 6 | 0 | -5.483500 | -2.947700 | -1.746500 |
| 6 | 6 | 0 | -6.292900 | -1.680200 | -1.452500 |
| 7 | 6 | 0 | -7.754400 | -2.024100 | -1.217700 |
| 8 | 6 | 0 | -2.506700 | -1.381400 | -3.742900 |
| 9 | 6 | 0 | -3.859900 | -4.077800 | -2.959600 |
| 10 | 6 | 0 | -5.132200 | -4.576000 | -3.243100 |
| 11 | 6 | 0 | -2.747000 | -4.751700 | -3.444400 |
| 12 | 6 | 0 | -2.937700 | -5.936500 | -4.167100 |
| 13 | 6 | 0 | -4.217000 | -6.423000 | -4.427800 |
| 14 | 6 | 0 | -5.347700 | -5.731600 | -3.968100 |
| 15 | 8 | 0 | -1.473500 | -4.316500 | -3.263700 |
| 16 | 8 | 0 | -6.121300 | -3.775000 | -2.736900 |
| 17 | 8 | 0 | -5.815500 | -1.161800 | -0.212700 |
| 18 | 6 | 0 | -4.395400 | -7.714600 | -5.186100 |
| 19 | 6 | 0 | -2.171700 | -1.701400 | -5.172900 |
| 20 | 6 | 0 | -1.589300 | -0.943900 | -2.873800 |
| 21 | 1 | 0 | -6.612000 | -1.006600 | -3.471600 |
| 22 | 1 | 0 | -6.664700 | 0.271500 | -2.248400 |
| 23 | 1 | 0 | -4.578500 | 0.444000 | -3.626700 |
| 24 | 1 | 0 | -4.156000 | 0.082000 | -1.970700 |
| 25 | 1 | 0 | -4.503200 | -1.956300 | -4.213100 |
| 26 | 1 | 0 | -3.353900 | -2.550700 | -1.456400 |
| 27 | 1 | 0 | -5.433300 | -3.525500 | -0.812400 |
| 28 | 1 | 0 | -8.298900 | -1.119400 | -0.935100 |
| 29 | 1 | 0 | -8.196700 | -2.452900 | -2.118300 |
| 30 | 1 | 0 | -7.839400 | -2.748000 | -0.403100 |
| 31 | 1 | 0 | -2.059900 | -6.461000 | -4.530100 |
| 32 | 1 | 0 | -6.352400 | -6.089900 | -4.162600 |
| 33 | 1 | 0 | -1.487300 | -3.417400 | -2.903500 |
| 34 | 1 | 0 | -4.902600 | -0.873800 | -0.328400 |
| 35 | 1 | 0 | -3.528200 | -7.928900 | -5.814300 |
| 36 | 1 | 0 | -4.522600 | -8.554500 | -4.495300 |
| 37 | 1 | 0 | -5.282100 | -7.676900 | -5.823900 |
| 38 | 1 | 0 | -2.772500 | -1.081100 | -5.847700 |
| 39 | 1 | 0 | -1.114800 | -1.537100 | -5.392600 |
| 40 | 1 | 0 | -2.419600 | -2.746300 | -5.393000 |
| 41 | 1 | 0 | -0.558300 | -0.781700 | -3.173000 |
| 42 | 1 | 0 | -1.840900 | -0.710800 | -1.842000 |

---

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 150.0353 Anisotropy = 19.4278

XX= 144.8057 YX= -0.5137 ZX= 2.5843

XY= -6.6060 YY= 156.0571 ZY= 9.2021

XZ= -3.1430 YZ= 9.1970 ZZ= 149.2430

Eigenvalues: 141.6389 145.4798 162.9872

2 C Isotropic = 157.6289 Anisotropy = 26.3532

XX= 169.4411 YX= -8.0872 ZX= 7.0245

XY= -3.9291 YY= 157.4212 ZY= -7.7871

XZ= 7.7114 YZ= -6.9767 ZZ= 146.0244

Eigenvalues: 141.7383 155.9506 175.1977

```
   3  C    Isotropic =   137.0466   Anisotropy =    10.7467
XX=   141.7862   YX=    -4.1890   ZX=    -0.6949
XY=     7.7834   YY=   141.9969   ZY=    -3.7685
XZ=     6.5195   YZ=    -7.4133   ZZ=   127.3566
Eigenvalues:   124.8096   142.1191   144.2110
   4  C    Isotropic =   135.8679   Anisotropy =    30.2510
XX=   125.9128   YX=     6.0119   ZX=     1.8153
XY=     5.5408   YY=   151.5066   ZY=    -2.1809
XZ=     8.4826   YZ=    18.6911   ZZ=   130.1843
Eigenvalues:   122.4718   129.0966   156.0352
   5  C    Isotropic =    95.3298   Anisotropy =    58.4343
XX=   119.1272   YX=    12.5445   ZX=   -20.0401
XY=     0.4439   YY=    85.8923   ZY=   -21.6635
XZ=   -26.3282   YZ=   -15.5518   ZZ=    80.9700
Eigenvalues:    61.0691    90.6344   134.2860
   6  C    Isotropic =   116.6755   Anisotropy =    54.1341
XX=   118.7115   YX=    10.3553   ZX=   -27.5192
XY=     8.8220   YY=   106.6614   ZY=   -11.8566
XZ=   -23.7312   YZ=   -12.8628   ZZ=   124.6534
Eigenvalues:    95.7056   101.5559   152.7649
   7  C    Isotropic =   161.2296   Anisotropy =    40.0028
XX=   149.6502   YX=   -10.6876   ZX=     0.0807
XY=    -7.8374   YY=   185.2284   ZY=    -3.2953
XZ=    -0.0748   YZ=    -4.8704   ZZ=   148.8102
Eigenvalues:   146.8046   148.9860   187.8981
   8  C    Isotropic =    16.6335   Anisotropy =   213.1559
XX=    39.4234   YX=    81.5062   ZX=   101.9432
XY=    83.8252   YY=   -26.6341   ZY=    -3.5562
XZ=    97.8451   YZ=     4.6562   ZZ=    37.1113
Eigenvalues:  -109.8532     1.0163   158.7375
   9  C    Isotropic =    68.8612   Anisotropy =   107.7717
XX=    23.5585   YX=    -1.4049   ZX=     8.0984
XY=   -16.9988   YY=    63.4065   ZY=    38.2758
XZ=    15.7797   YZ=    41.6234   ZZ=   119.6186
Eigenvalues:    16.1801    49.6945   140.7090
  10  C    Isotropic =    20.5390   Anisotropy =   110.4394
XX=   -32.5489   YX=    32.2027   ZX=    -5.5464
XY=    42.9564   YY=    12.1693   ZY=    36.7523
XZ=   -16.4449   YZ=    26.1455   ZZ=    81.9966
Eigenvalues:   -58.5736    26.0254    94.1653
  11  C    Isotropic =    28.2141   Anisotropy =   135.2692
XX=    15.3466   YX=    -6.3573   ZX=     9.5344
XY=     0.2165   YY=   -25.1764   ZY=    61.8866
XZ=     5.6104   YZ=    54.3642   ZZ=    94.4720
Eigenvalues:   -49.2669    15.5156   118.3935
  12  C    Isotropic =    74.5480   Anisotropy =   117.1399
XX=    20.3988   YX=    29.1280   ZX=    -4.3131
XY=    40.5163   YY=    62.2443   ZY=    37.8512
XZ=    -7.0798   YZ=    25.9957   ZZ=   141.0008
Eigenvalues:    -2.4456    73.4483   152.6412
  13  C    Isotropic =    40.7650   Anisotropy =   194.5100
XX=   -41.8461   YX=   -16.3708   ZX=    20.3316
```

```
XY=   -18.6398   YY=    29.2500   ZY=    67.4719
XZ=    28.2846   YZ=    71.8671   ZZ=   134.8912
Eigenvalues:   -56.4483     8.3051   170.4384
  14  C    Isotropic =    80.9841   Anisotropy =   121.1414
XX=    74.6237   YX=     9.3520   ZX=     1.9367
XY=    -7.1553   YY=    33.0883   ZY=    61.0813
XZ=     1.9743   YZ=    55.5570   ZZ=   135.2403
Eigenvalues:     6.6404    74.5669   161.7451
  15  O    Isotropic =   203.4951   Anisotropy =    75.0674
XX=   148.2851   YX=    12.8148   ZX=    -0.4643
XY=     5.8899   YY=   211.4176   ZY=    10.9964
XZ=    23.1247   YZ=   -28.9472   ZZ=   250.7826
Eigenvalues:   145.4342   211.5110   253.5401
  16  O    Isotropic =   186.1491   Anisotropy =   115.9842
XX=   222.4768   YX=   -60.8667   ZX=    36.2135
XY=   -45.1846   YY=   150.6954   ZY=    32.4912
XZ=    33.2928   YZ=   -35.4012   ZZ=   185.2751
Eigenvalues:   118.7437   176.2318   263.4719
  17  O    Isotropic =   255.8379   Anisotropy =    40.1149
XX=   274.5035   YX=     7.2516   ZX=   -18.8750
XY=     1.4444   YY=   243.8149   ZY=    -6.2803
XZ=    -9.9755   YZ=   -11.5213   ZZ=   249.1953
Eigenvalues:   236.2729   248.6597   282.5812
  18  C    Isotropic =   163.7743   Anisotropy =    41.3209
XX=   184.7824   YX=     8.5175   ZX=   -11.4609
XY=    13.0585   YY=   158.7669   ZY=   -10.5878
XZ=    -5.0775   YZ=    -6.3240   ZZ=   147.7735
Eigenvalues:   143.0477   156.9536   191.3216
  19  C    Isotropic =   157.9337   Anisotropy =    42.5426
XX=   159.5410   YX=   -15.3203   ZX=   -17.3990
XY=   -11.9726   YY=   159.2293   ZY=     8.7972
XZ=   -19.0395   YZ=    11.5600   ZZ=   155.0308
Eigenvalues:   138.7703   148.7354   186.2954
  20  C    Isotropic =    72.6365   Anisotropy =   130.3311
XX=    86.6411   YX=    76.5590   ZX=    49.7766
XY=    73.2595   YY=    27.9178   ZY=   -15.8162
XZ=    50.6160   YZ=   -18.6724   ZZ=   103.3507
Eigenvalues:   -36.6554    95.0411   159.5239
  21  H    Isotropic =    30.0824   Anisotropy =     6.2576
XX=    27.1770   YX=    -0.8878   ZX=    -0.9271
XY=     0.0081   YY=    29.3209   ZY=    -1.3477
XZ=     0.3654   YZ=    -1.7996   ZZ=    33.7494
Eigenvalues:    27.0321    28.9610    34.2542
  22  H    Isotropic =    30.0888   Anisotropy =     8.9476
XX=    33.7462   YX=    -2.1171   ZX=     3.9007
XY=    -1.7378   YY=    29.2914   ZY=     0.3984
XZ=     4.1367   YZ=     0.1783   ZZ=    27.2289
Eigenvalues:    25.0190    29.1936    36.0539
  23  H    Isotropic =    30.2267   Anisotropy =     9.6251
XX=    29.6950   YX=     0.7709   ZX=     3.9715
XY=     1.0427   YY=    30.8101   ZY=     4.3814
XZ=     4.2695   YZ=     4.1354   ZZ=    30.1749
```

```
Eigenvalues:    24.7017    29.3349    36.6434
  24  H    Isotropic =    30.5199   Anisotropy =     6.2664
XX=    31.5030   YX=     1.5713   ZX=    -2.3980
XY=     1.7863   YY=    32.5400   ZY=    -2.0940
XZ=    -1.4427   YZ=    -1.4318   ZZ=    27.5166
Eigenvalues:    26.5447    30.3175    34.6975
  25  H    Isotropic =    30.0948   Anisotropy =     3.7695
XX=    30.7223   YX=    -1.7589   ZX=    -2.4292
XY=    -0.1066   YY=    29.6909   ZY=     0.4402
XZ=    -0.0699   YZ=     2.6530   ZZ=    29.8710
Eigenvalues:    28.2133    29.4633    32.6077
  26  H    Isotropic =    28.8444   Anisotropy =     4.3420
XX=    27.7896   YX=    -0.0986   ZX=     0.2900
XY=    -1.8517   YY=    29.3083   ZY=    -2.0580
XZ=    -0.8565   YZ=    -2.5544   ZZ=    29.4354
Eigenvalues:    26.4464    28.3478    31.7391
  27  H    Isotropic =    27.6248   Anisotropy =     4.7471
XX=    26.8325   YX=     0.6846   ZX=    -1.1007
XY=    -0.8749   YY=    27.6341   ZY=     0.9070
XZ=    -3.3178   YZ=     2.7926   ZZ=    28.4077
Eigenvalues:    24.8507    27.2341    30.7895
  28  H    Isotropic =    30.6019   Anisotropy =     9.4927
XX=    34.0019   YX=    -3.3031   ZX=     1.8958
XY=    -4.3166   YY=    30.8329   ZY=    -0.8105
XZ=     1.8718   YZ=    -0.6067   ZZ=    26.9709
Eigenvalues:    26.4747    28.4006    36.9303
  29  H    Isotropic =    30.2820   Anisotropy =     8.0990
XX=    29.5121   YX=     0.1222   ZX=    -1.9979
XY=     0.3687   YY=    32.2787   ZY=    -4.6104
XZ=    -1.8337   YZ=    -4.2844   ZZ=    29.0554
Eigenvalues:    25.4174    29.7474    35.6814
  30  H    Isotropic =    30.4357   Anisotropy =     9.4216
XX=    27.7370   YX=    -1.0096   ZX=     0.0206
XY=    -0.8138   YY=    34.4417   ZY=     4.5694
XZ=     0.0863   YZ=     3.5805   ZZ=    29.1285
Eigenvalues:    26.6866    27.9037    36.7168
  31  H    Isotropic =    25.2796   Anisotropy =     6.7903
XX=    27.0518   YX=     2.3768   ZX=    -0.9907
XY=     2.5049   YY=    26.3363   ZY=    -2.3167
XZ=    -0.7375   YZ=    -2.2390   ZZ=    22.4508
Eigenvalues:    21.3873    24.6450    29.8065
  32  H    Isotropic =    25.3585   Anisotropy =     7.3695
XX=    30.0830   YX=     0.5273   ZX=    -0.7565
XY=     0.9817   YY=    24.1566   ZY=    -1.3285
XZ=    -0.6320   YZ=    -1.6416   ZZ=    21.8359
Eigenvalues:    21.1018    24.7022    30.2715
  33  H    Isotropic =    26.5623   Anisotropy =    16.7927
XX=    35.2056   YX=     4.2326   ZX=     3.4267
XY=     6.0764   YY=    26.3538   ZY=    -2.7500
XZ=     2.1552   YZ=    -0.4139   ZZ=    18.1276
Eigenvalues:    16.9887    24.9409    37.7575
  34  H    Isotropic =    30.5434   Anisotropy =    14.8086
```

```
XX=    24.9320   YX=    -0.8901   ZX=    -3.8390
XY=    -0.8458   YY=    38.2640   ZY=    -4.6468
XZ=    -4.9862   YZ=    -5.3463   ZZ=    28.4343
Eigenvalues:    21.1504    30.0640    40.4158
  35  H    Isotropic =    29.7239   Anisotropy =     7.9436
XX=    33.8201   YX=    -3.0822   ZX=    -1.6299
XY=    -1.0300   YY=    29.8960   ZY=    -0.8898
XZ=    -2.7235   YZ=    -0.5790   ZZ=    25.4555
Eigenvalues:    24.6296    29.5224    35.0196
  36  H    Isotropic =    29.3154   Anisotropy =     9.1322
XX=    30.6373   YX=     3.5028   ZX=     1.8482
XY=     3.7184   YY=    29.8947   ZY=     2.0887
XZ=     2.9927   YZ=     2.9045   ZZ=    27.4143
Eigenvalues:    25.8498    26.6929    35.4036
  37  H    Isotropic =    29.6121   Anisotropy =     7.8575
XX=    30.1271   YX=     1.9750   ZX=    -2.1098
XY=     0.1175   YY=    28.5395   ZY=    -4.3455
XZ=    -1.3254   YZ=    -4.8250   ZZ=    30.1696
Eigenvalues:    24.6793    29.3065    34.8504
  38  H    Isotropic =    30.0472   Anisotropy =     8.0146
XX=    27.3877   YX=    -0.8313   ZX=     0.5925
XY=    -1.0667   YY=    28.3420   ZY=     2.7398
XZ=     1.0392   YZ=     2.4369   ZZ=    34.4121
Eigenvalues:    26.2049    28.5465    35.3903
  39  H    Isotropic =    29.9702   Anisotropy =     8.7914
XX=    28.2666   YX=    -3.8294   ZX=    -0.7519
XY=    -2.2051   YY=    34.2501   ZY=    -0.0815
XZ=    -1.4031   YZ=     2.7593   ZZ=    27.3940
Eigenvalues:    26.5680    27.5115    35.8312
  40  H    Isotropic =    30.0024   Anisotropy =     5.8166
XX=    32.2424   YX=     2.4284   ZX=    -1.3491
XY=     1.9018   YY=    30.2026   ZY=     2.3265
XZ=    -0.2233   YZ=     4.1539   ZZ=    27.5624
Eigenvalues:    24.8961    31.2310    33.8802
  41  H    Isotropic =    26.3381   Anisotropy =     5.5578
XX=    25.2191   YX=     3.0276   ZX=    -1.1313
XY=     1.0753   YY=    27.6087   ZY=    -1.2238
XZ=     0.1865   YZ=    -3.2542   ZZ=    26.1866
Eigenvalues:    23.7154    25.2556    30.0433
  42  H    Isotropic =    26.4552   Anisotropy =     8.2378
XX=    24.9954   YX=     0.6775   ZX=     0.4463
XY=     3.4080   YY=    28.5370   ZY=    -5.9718
XZ=    -0.6816   YZ=    -2.2473   ZZ=    25.8333
Eigenvalues:    22.3382    25.0804    31.9471
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 56.85 | 72.14 | 86.16 | 94.91 | 122.22 | 129.94 |
| intensities | 1.38 | 1.31 | 0.86 | 0.27 | 1.03 | 2.29 |
| reduc. mass | 1.14 | 0.96 | 0.45 | 1.16 | 1.06 | 0.93 |
| force const | 0.00 | 0.00 | 0.00 | 0.01 | 0.01 | 0.01 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 165.43 | 193.26 | 221.77 | 224.22 | 251.72 | 257.75 |
| intensities | 0.67 | 0.11 | 0.15 | 7.58 | 3.81 | 3.75 |
| reduc. mass | 0.83 | 0.64 | 1.45 | 0.34 | 1.23 | 0.99 |
| force const | 0.01 | 0.01 | 0.04 | 0.01 | 0.05 | 0.04 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 265.60 | 270.84 | 303.31 | 311.25 | 326.97 | 330.26 |
| intensities | 5.10 | 5.06 | 1.84 | 4.80 | 0.47 | 5.20 |
| reduc. mass | 0.33 | 0.93 | 0.82 | 1.03 | 0.20 | 1.65 |
| force const | 0.01 | 0.04 | 0.04 | 0.06 | 0.01 | 0.11 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 365.20 | 385.90 | 401.10 | 440.10 | 471.49 | 490.54 |
| intensities | 2.94 | 20.42 | 1.44 | 5.49 | 3.67 | 11.15 |
| reduc. mass | 0.36 | 0.30 | 0.68 | 0.96 | 0.60 | 1.07 |
| force const | 0.03 | 0.03 | 0.06 | 0.11 | 0.08 | 0.15 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 514.99 | 526.36 | 532.15 | 547.60 | 566.37 | 600.36 |
| intensities | 0.65 | 8.80 | 7.43 | 6.70 | 33.22 | 19.35 |
| reduc. mass | 0.51 | 0.76 | 0.81 | 0.63 | 0.53 | 2.05 |
| force const | 0.08 | 0.12 | 0.13 | 0.11 | 0.10 | 0.43 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 653.14 | 665.37 | 693.48 | 708.85 | 715.36 | 732.50 |
| intensities | 80.43 | 26.78 | 13.31 | 13.18 | 1.00 | 3.68 |
| reduc. mass | 0.52 | 0.77 | 1.49 | 2.30 | 0.39 | 0.57 |
| force const | 0.13 | 0.20 | 0.42 | 0.68 | 0.12 | 0.18 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 749.90 | 808.72 | 833.24 | 848.43 | 866.97 | 920.49 |
| intensities | 7.36 | 1.36 | 4.53 | 2.12 | 5.12 | 1.13 |
| reduc. mass | 1.21 | 1.19 | 1.59 | 0.63 | 0.63 | 0.87 |
| force const | 0.40 | 0.46 | 0.65 | 0.27 | 0.28 | 0.43 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 936.72 | 947.90 | 955.98 | 997.06 | 1012.08 | 1013.23 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 7.34 | 1.01 | 17.34 | 3.67 | 5.58 | 4.10 |
| reduc. mass | 0.66 | 0.76 | 0.44 | 0.28 | 0.26 | 0.21 |
| force const | 0.34 | 0.40 | 0.23 | 0.16 | 0.15 | 0.13 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1030.67 | 1049.21 | 1054.67 | 1060.39 | 1063.37 | 1093.64 |
| intensities | 20.18 | 12.01 | 6.20 | 20.64 | 24.28 | 13.46 |
| reduc. mass | 0.52 | 0.31 | 0.46 | 0.30 | 0.53 | 0.41 |
| force const | 0.33 | 0.20 | 0.30 | 0.20 | 0.35 | 0.29 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1103.40 | 1111.00 | 1137.26 | 1148.18 | 1163.67 | 1224.61 |
| intensities | 42.09 | 95.53 | 7.68 | 44.05 | 5.14 | 29.32 |
| reduc. mass | 0.72 | 0.50 | 0.47 | 0.75 | 0.65 | 0.41 |
| force const | 0.51 | 0.36 | 0.36 | 0.59 | 0.52 | 0.36 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1228.67 | 1250.32 | 1255.20 | 1288.33 | 1302.85 | 1320.25 |
| intensities | 57.10 | 31.93 | 65.43 | 29.31 | 54.42 | 81.12 |
| reduc. mass | 0.57 | 0.28 | 0.68 | 0.93 | 0.63 | 0.98 |
| force const | 0.51 | 0.25 | 0.63 | 0.91 | 0.63 | 1.00 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1337.86 | 1386.51 | 1401.48 | 1410.79 | 1433.94 | 1473.79 |
| intensities | 40.85 | 85.38 | 110.33 | 443.63 | 90.55 | 17.51 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.90 | 0.61 | 0.36 | 0.64 | 0.54 | 1.61 |
| force const | 0.95 | 0.69 | 0.42 | 0.75 | 0.65 | 2.07 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1499.76 | 1510.00 | 1513.68 | 1523.65 | 1528.26 | 1531.71 |
| intensities | 0.80 | 25.43 | 130.97 | 1.02 | 69.76 | 6.26 |
| reduc. mass | 0.93 | 2.19 | 1.26 | 2.72 | 0.73 | 0.48 |
| force const | 1.23 | 2.94 | 1.71 | 3.71 | 1.01 | 0.67 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1565.30 | 1581.11 | 1587.62 | 1624.61 | 1638.08 | 1641.91 |
| intensities | 110.26 | 19.56 | 24.11 | 9.43 | 99.92 | 47.35 |
| reduc. mass | 0.76 | 0.63 | 0.42 | 0.44 | 0.20 | 0.35 |
| force const | 1.10 | 0.92 | 0.62 | 0.69 | 0.31 | 0.55 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1651.11 | 1656.37 | 1660.58 | 1662.18 | 1665.04 | 1669.93 |
| intensities | 62.42 | 5.93 | 31.90 | 30.15 | 20.69 | 4.64 |
| reduc. mass | 0.14 | 0.85 | 0.28 | 0.36 | 0.27 | 0.26 |
| force const | 0.23 | 1.38 | 0.45 | 0.59 | 0.45 | 0.42 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1675.92 | 1678.37 | 1679.52 | 1679.79 | 1683.52 | 1808.57 |
| intensities | 106.06 | 41.11 | 29.71 | 3.88 | 12.82 | 869.62 |
| reduc. mass | 0.56 | 0.21 | 0.14 | 0.16 | 0.28 | 1.60 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 0.93 | 0.35 | 0.24 | 0.27 | 0.46 | 3.09 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1837.16 | 1888.57 | 3020.26 | 3028.18 | 3034.88 | 3048.97 |
| intensities | 377.99 | 14.50 | 296.20 | 537.30 | 592.61 | 371.59 |
| reduc. mass | 1.37 | 0.86 | 0.33 | 0.16 | 0.14 | 0.39 |
| force const | 2.73 | 1.81 | 1.75 | 0.88 | 0.78 | 2.15 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3060.09 | 3074.68 | 3078.03 | 3088.89 | 3108.89 | 3118.67 |
| intensities | 534.78 | 349.03 | 118.08 | 248.24 | 311.50 | 247.29 |
| reduc. mass | 0.30 | 0.88 | 0.75 | 0.77 | 0.27 | 0.54 |
| force const | 1.66 | 4.87 | 4.21 | 4.33 | 1.54 | 3.11 |

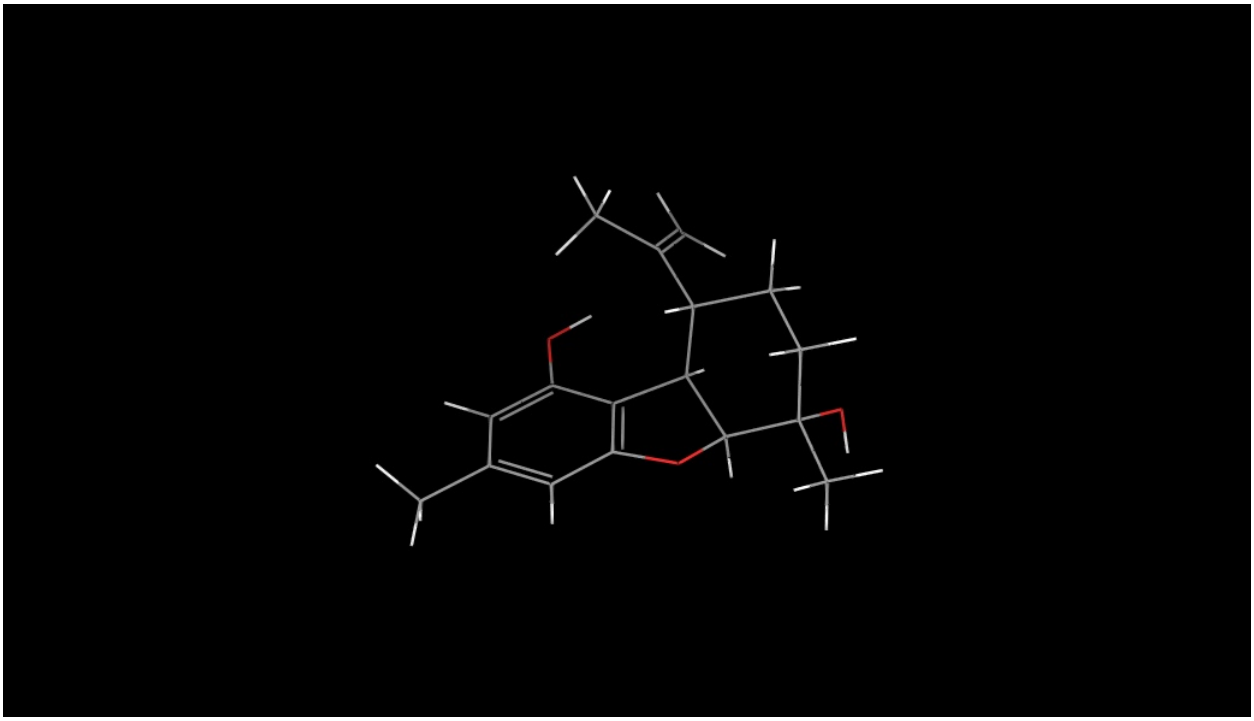
| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3123.92 | 3130.77 | 3135.84 | 3145.40 | 3146.48 | 3147.59 |
| intensities | 343.40 | 498.32 | 448.61 | 429.34 | 346.32 | 186.55 |
| reduc. mass | 0.50 | 0.45 | 0.50 | 0.21 | 0.22 | 0.20 |
| force const | 2.88 | 2.62 | 2.89 | 1.25 | 1.26 | 1.16 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3154.94 | 3155.63 | 3179.13 | 3196.86 | 3825.64 | 3856.43 |
| intensities | 403.96 | 529.07 | 96.06 | 334.19 | 74.43 | 69.56 |
| reduc. mass | 0.31 | 0.28 | 0.33 | 0.52 | 0.95 | 0.95 |
| force const | 1.84 | 1.64 | 1.95 | 3.12 | 8.17 | 8.30 |

Number of imaginary frequencies: 0

Conformation 6

Boltzmann Population = 41.4% (relative energy = 0.00 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.983252 hartrees

Total enthalpy, Htot (Utot + pV): -885.982308 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.044598 hartrees

Optimized geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -6.008100 | -0.538700 | -2.669400 |
| 2 | 6 | 0 | -4.530500 | -0.281400 | -2.962800 |
| 3 | 6 | 0 | -3.864200 | -1.584400 | -3.418300 |
| 4 | 6 | 0 | -3.981700 | -2.685700 | -2.336700 |
| 5 | 6 | 0 | -5.410800 | -2.837300 | -1.783000 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 6 | 0 | -6.185000 | -1.540200 | -1.529600 |
| 7 | 6 | 0 | -7.655800 | -1.835800 | -1.264300 |
| 8 | 6 | 0 | -2.415700 | -1.412400 | -3.845000 |
| 9 | 6 | 0 | -3.834800 | -4.051200 | -2.970900 |
| 10 | 6 | 0 | -5.120800 | -4.532100 | -3.215100 |
| 11 | 6 | 0 | -2.745800 | -4.769300 | -3.450000 |
| 12 | 6 | 0 | -2.975400 | -5.974700 | -4.124600 |
| 13 | 6 | 0 | -4.269700 | -6.442100 | -4.346000 |
| 14 | 6 | 0 | -5.375500 | -5.709300 | -3.893000 |
| 15 | 8 | 0 | -1.460500 | -4.357100 | -3.305600 |
| 16 | 8 | 0 | -6.086300 | -3.692600 | -2.720900 |
| 17 | 8 | 0 | -5.581700 | -0.923200 | -0.393500 |
| 18 | 6 | 0 | -4.482400 | -7.757900 | -5.052900 |
| 19 | 6 | 0 | -2.100200 | -1.771500 | -5.270400 |
| 20 | 6 | 0 | -1.480400 | -0.984100 | -2.990400 |
| 21 | 1 | 0 | -6.505400 | -0.933600 | -3.563700 |
| 22 | 1 | 0 | -6.518000 | 0.386500 | -2.382600 |
| 23 | 1 | 0 | -4.422300 | 0.476900 | -3.745200 |
| 24 | 1 | 0 | -4.039000 | 0.103500 | -2.063000 |
| 25 | 1 | 0 | -4.428800 | -1.945300 | -4.289600 |
| 26 | 1 | 0 | -3.283800 | -2.478500 | -1.519300 |
| 27 | 1 | 0 | -5.355100 | -3.388000 | -0.828300 |
| 28 | 1 | 0 | -8.176600 | -0.908500 | -1.012100 |
| 29 | 1 | 0 | -8.123800 | -2.291400 | -2.139000 |
| 30 | 1 | 0 | -7.762400 | -2.535900 | -0.427200 |
| 31 | 1 | 0 | -2.115800 | -6.532000 | -4.482800 |
| 32 | 1 | 0 | -6.391200 | -6.050700 | -4.058000 |
| 33 | 1 | 0 | -1.448900 | -3.443900 | -2.981100 |
| 34 | 1 | 0 | -5.792300 | -1.456300 | 0.382800 |
| 35 | 1 | 0 | -3.719200 | -7.923800 | -5.817000 |
| 36 | 1 | 0 | -4.428900 | -8.591900 | -4.345600 |
| 37 | 1 | 0 | -5.462800 | -7.793300 | -5.533500 |
| 38 | 1 | 0 | -2.689900 | -1.150300 | -5.954200 |
| 39 | 1 | 0 | -1.041200 | -1.639700 | -5.501600 |
| 40 | 1 | 0 | -2.377000 | -2.814000 | -5.466700 |
| 41 | 1 | 0 | -0.447800 | -0.855800 | -3.301000 |
| 42 | 1 | 0 | -1.722100 | -0.720100 | -1.963900 |

---

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 150.7318 Anisotropy = 20.3115

XX= 144.4025 YX= -1.1717 ZX= 1.6644

XY= -7.1709 YY= 159.8624 ZY= 6.4984

XZ= -3.1305 YZ= 8.3820 ZZ= 147.9306

Eigenvalues: 142.7729 145.1498 164.2728

2 C Isotropic = 157.7964 Anisotropy = 22.0893

XX= 166.4161 YX= -7.0108 ZX= 6.4954

XY= -3.0676 YY= 160.8227 ZY= -6.4388

XZ= 7.0999 YZ= -6.1598 ZZ= 146.1505

```
Eigenvalues:   142.8058   158.0608   172.5226
   3  C    Isotropic =   135.8320   Anisotropy =    10.4231
XX=   141.4309   YX=    -4.1984   ZX=    -0.4463
XY=     7.7029   YY=   140.1081   ZY=    -4.1254
XZ=     6.3122   YZ=    -7.5672   ZZ=   125.9568
Eigenvalues:   123.2354   141.4798   142.7807
   4  C    Isotropic =   135.2984   Anisotropy =    28.8697
XX=   126.4414   YX=     5.4492   ZX=     1.8969
XY=     3.8807   YY=   151.3987   ZY=    -3.3826
XZ=     7.4689   YZ=    17.4455   ZZ=   128.0551
Eigenvalues:   122.4534   128.8969   154.5449
   5  C    Isotropic =    93.8077   Anisotropy =    55.7736
XX=   117.1413   YX=    10.6470   ZX=   -20.2736
XY=     0.3793   YY=    84.6059   ZY=   -20.7601
XZ=   -24.5553   YZ=   -12.9470   ZZ=    79.6760
Eigenvalues:    61.2750    89.1580   130.9901
   6  C    Isotropic =   116.3215   Anisotropy =    53.0090
XX=   118.0769   YX=     8.3309   ZX=   -26.2986
XY=     6.3311   YY=   107.5860   ZY=   -12.7957
XZ=   -24.4627   YZ=   -15.6120   ZZ=   123.3015
Eigenvalues:    93.4481   103.8555   151.6608
   7  C    Isotropic =   157.5827   Anisotropy =    45.0814
XX=   142.0945   YX=   -12.0793   ZX=     0.6310
XY=    -8.2999   YY=   184.6803   ZY=    -5.2990
XZ=     0.1800   YZ=    -5.1398   ZZ=   145.9734
Eigenvalues:   139.6811   145.4300   187.6370
   8  C    Isotropic =    16.8070   Anisotropy =   212.5285
XX=    42.3345   YX=    82.0505   ZX=   101.2864
XY=    84.0022   YY=   -26.9393   ZY=    -5.0861
XZ=    96.9523   YZ=     3.4360   ZZ=    35.0258
Eigenvalues:  -109.8143     1.7427   158.4927
   9  C    Isotropic =    68.3533   Anisotropy =   110.4661
XX=    22.1158   YX=    -0.1874   ZX=     8.1954
XY=   -16.1560   YY=    62.3881   ZY=    38.8437
XZ=    15.6726   YZ=    42.8100   ZZ=   120.5560
Eigenvalues:    15.4766    47.5859   141.9973
  10  C    Isotropic =    20.6697   Anisotropy =   109.4695
XX=   -32.9708   YX=    32.2433   ZX=    -4.9079
XY=    43.8546   YY=    12.8073   ZY=    35.3793
XZ=   -16.4067   YZ=    25.2227   ZZ=    82.1726
Eigenvalues:   -58.7828    27.1425    93.6494
  11  C    Isotropic =    27.8218   Anisotropy =   135.8125
XX=    14.8135   YX=    -6.4728   ZX=     9.6410
XY=     0.5065   YY=   -26.2665   ZY=    61.3597
XZ=     5.7699   YZ=    54.0791   ZZ=    94.9184
Eigenvalues:   -49.8500    14.9520   118.3634
  12  C    Isotropic =    74.4502   Anisotropy =   119.7983
XX=    19.3315   YX=    28.0171   ZX=    -3.3577
XY=    40.6991   YY=    61.3072   ZY=    38.2882
XZ=    -6.7721   YZ=    26.3148   ZZ=   142.7118
Eigenvalues:    -2.9109    71.9457   154.3157
  13  C    Isotropic =    41.2810   Anisotropy =   193.7540
```

```
XX=   -41.3722   YX=   -16.4601   ZX=    20.3882
XY=   -18.8872   YY=    29.2994   ZY=    66.4127
XZ=    28.5426   YZ=    70.7707   ZZ=   135.9159
Eigenvalues:   -55.9784     9.3711   170.4504
  14  C    Isotropic =    81.0701   Anisotropy =   118.2327
XX=    76.5406   YX=     8.5783   ZX=     2.1664
XY=    -6.3374   YY=    32.2329   ZY=    59.6442
XZ=     1.2704   YZ=    54.2338   ZZ=   134.4366
Eigenvalues:     6.8255    76.4929   159.8919
  15  O    Isotropic =   202.8541   Anisotropy =    76.2079
XX=   147.0289   YX=    12.3294   ZX=    -0.0912
XY=     6.0680   YY=   210.7244   ZY=    11.0274
XZ=    23.5322   YZ=   -29.2768   ZZ=   250.8089
Eigenvalues:   144.1589   210.7440   253.6593
  16  O    Isotropic =   185.1597   Anisotropy =   111.4585
XX=   219.9163   YX=   -59.2466   ZX=    34.2889
XY=   -42.9511   YY=   148.9566   ZY=    32.5390
XZ=    32.6213   YZ=   -35.1346   ZZ=   186.6062
Eigenvalues:   118.8279   177.1858   259.4654
  17  O    Isotropic =   244.0193   Anisotropy =    66.8163
XX=   225.0180   YX=    10.4561   ZX=    -6.1564
XY=    11.2197   YY=   224.6959   ZY=    21.5940
XZ=   -21.9855   YZ=    10.9539   ZZ=   282.3441
Eigenvalues:   207.8272   235.6673   288.5636
  18  C    Isotropic =   163.8245   Anisotropy =    41.3368
XX=   183.5806   YX=    10.7827   ZX=   -12.4792
XY=    12.4814   YY=   160.0542   ZY=   -11.1444
XZ=    -4.7383   YZ=    -6.8256   ZZ=   147.8387
Eigenvalues:   142.9321   157.1591   191.3824
  19  C    Isotropic =   157.9363   Anisotropy =    42.5616
XX=   158.8621   YX=   -15.4742   ZX=   -17.2884
XY=   -12.1701   YY=   159.7247   ZY=     8.8072
XZ=   -18.9679   YZ=    11.6738   ZZ=   155.2222
Eigenvalues:   138.6081   148.8901   186.3107
  20  C    Isotropic =    72.1289   Anisotropy =   131.1515
XX=    88.6283   YX=    76.8692   ZX=    48.9183
XY=    73.3836   YY=    25.4489   ZY=   -15.6382
XZ=    49.9092   YZ=   -18.4472   ZZ=   102.3093
Eigenvalues:   -37.3426    94.1660   159.5632
  21  H    Isotropic =    30.2441   Anisotropy =     6.2210
XX=    27.4535   YX=    -0.9283   ZX=    -0.8246
XY=     0.1570   YY=    29.4561   ZY=    -1.6097
XZ=     0.4580   YZ=    -1.7399   ZZ=    33.8227
Eigenvalues:    27.3372    29.0037    34.3914
  22  H    Isotropic =    30.0073   Anisotropy =     8.8909
XX=    33.6975   YX=    -2.0262   ZX=     3.8459
XY=    -1.7683   YY=    29.1238   ZY=     0.4953
XZ=     4.0760   YZ=     0.2395   ZZ=    27.2008
Eigenvalues:    24.9915    29.0960    35.9346
  23  H    Isotropic =    30.4389   Anisotropy =     9.5140
XX=    30.0525   YX=     0.7232   ZX=     3.9097
XY=     1.0903   YY=    31.3331   ZY=     4.4730
```

```
XZ=     4.3185   YZ=     4.0286   ZZ=    29.9312
Eigenvalues:    24.7679    29.7674    36.7816
  24  H    Isotropic =    29.7989   Anisotropy =     5.9477
XX=    30.5253   YX=     1.1890   ZX=    -2.7691
XY=     1.4919   YY=    31.6640   ZY=    -2.0410
XZ=    -1.8403   YZ=    -1.5638   ZZ=    27.2074
Eigenvalues:    25.8347    29.7979    33.7640
  25  H    Isotropic =    30.1068   Anisotropy =     3.8612
XX=    30.6548   YX=    -1.8009   ZX=    -2.3142
XY=    -0.2856   YY=    29.7693   ZY=     0.5259
XZ=    -0.0107   YZ=     2.7618   ZZ=    29.8964
Eigenvalues:    28.1861    29.4535    32.6809
  26  H    Isotropic =    28.5368   Anisotropy =     4.3769
XX=    27.3277   YX=    -0.1022   ZX=     0.0266
XY=    -1.8486   YY=    29.0828   ZY=    -2.0647
XZ=    -0.9463   YZ=    -2.4974   ZZ=    29.1997
Eigenvalues:    26.0387    28.1169    31.4547
  27  H    Isotropic =    27.9439   Anisotropy =     4.8050
XX=    27.1945   YX=     0.6750   ZX=    -1.2891
XY=    -0.7690   YY=    27.9835   ZY=     0.8067
XZ=    -3.5722   YZ=     2.6905   ZZ=    28.6538
Eigenvalues:    24.9987    27.6859    31.1473
  28  H    Isotropic =    30.5168   Anisotropy =     9.0632
XX=    33.5338   YX=    -3.1093   ZX=     1.8264
XY=    -4.3899   YY=    30.8297   ZY=    -0.7110
XZ=     2.0002   YZ=    -0.4885   ZZ=    27.1869
Eigenvalues:    26.5772    28.4143    36.5590
  29  H    Isotropic =    29.9765   Anisotropy =     8.3836
XX=    28.9740   YX=     0.0348   ZX=    -1.8442
XY=     0.5456   YY=    32.1640   ZY=    -4.8022
XZ=    -1.8320   YZ=    -4.2487   ZZ=    28.7914
Eigenvalues:    25.1541    29.2097    35.5655
  30  H    Isotropic =    30.8405   Anisotropy =     8.9663
XX=    28.4609   YX=    -0.9631   ZX=    -0.1448
XY=    -0.7818   YY=    34.8995   ZY=     4.3305
XZ=    -0.0047   YZ=     3.1350   ZZ=    29.1611
Eigenvalues:    27.2345    28.4689    36.8181
  31  H    Isotropic =    25.2584   Anisotropy =     6.9009
XX=    26.9646   YX=     2.4840   ZX=    -1.0410
XY=     2.5268   YY=    26.3914   ZY=    -2.3135
XZ=    -0.7633   YZ=    -2.2234   ZZ=    22.4193
Eigenvalues:    21.3800    24.5362    29.8590
  32  H    Isotropic =    25.3925   Anisotropy =     7.2456
XX=    30.0305   YX=     0.5218   ZX=    -0.7686
XY=     0.9750   YY=    24.2472   ZY=    -1.3366
XZ=    -0.6289   YZ=    -1.6526   ZZ=    21.8999
Eigenvalues:    21.1627    24.7919    30.2230
  33  H    Isotropic =    26.3820   Anisotropy =    17.1454
XX=    35.1996   YX=     4.3309   ZX=     3.4812
XY=     6.1823   YY=    26.1427   ZY=    -2.6675
XZ=     2.2571   YZ=    -0.2893   ZZ=    17.8038
Eigenvalues:    16.6974    24.6364    37.8123
```

```
  34  H    Isotropic =    31.8068   Anisotropy =    16.4417
XX=    27.0866   YX=     0.4294   ZX=    -4.5672
XY=    -0.3407   YY=    29.6988   ZY=     5.7124
XZ=    -4.0003   YZ=     6.7570   ZZ=    38.6350
Eigenvalues:    24.3800    28.2724    42.7680
  35  H    Isotropic =    29.5858   Anisotropy =     8.0538
XX=    33.1532   YX=    -2.8201   ZX=    -2.5616
XY=    -1.1071   YY=    29.7335   ZY=    -0.2366
XZ=    -3.7019   YZ=     0.1102   ZZ=    25.8708
Eigenvalues:    24.5945    29.2080    34.9550
  36  H    Isotropic =    29.3194   Anisotropy =     9.1628
XX=    31.0336   YX=     3.2349   ZX=     2.4839
XY=     3.8767   YY=    28.8095   ZY=     1.6703
XZ=     3.5751   YZ=     2.2688   ZZ=    28.1151
Eigenvalues:    26.0665    26.4638    35.4279
  37  H    Isotropic =    29.7561   Anisotropy =     7.7114
XX=    30.3136   YX=     2.1221   ZX=    -1.8961
XY=     0.0305   YY=    29.8918   ZY=    -4.5934
XZ=    -0.9172   YZ=    -4.8801   ZZ=    29.0630
Eigenvalues:    24.7044    29.6669    34.8971
  38  H    Isotropic =    30.0408   Anisotropy =     7.9947
XX=    27.3940   YX=    -0.7979   ZX=     0.7091
XY=    -1.0595   YY=    28.3935   ZY=     2.7844
XZ=     1.1443   YZ=     2.4807   ZZ=    34.3350
Eigenvalues:    26.1816    28.5703    35.3706
  39  H    Isotropic =    29.9846   Anisotropy =     8.7650
XX=    28.2135   YX=    -3.7602   ZX=    -0.7111
XY=    -2.1772   YY=    34.3112   ZY=    -0.1064
XZ=    -1.3586   YZ=     2.7449   ZZ=    27.4291
Eigenvalues:    26.6057    27.5201    35.8280
  40  H    Isotropic =    30.0084   Anisotropy =     5.6581
XX=    32.2579   YX=     2.3756   ZX=    -1.4049
XY=     1.8416   YY=    30.1565   ZY=     2.2932
XZ=    -0.2799   YZ=     4.0466   ZZ=    27.6107
Eigenvalues:    24.9682    31.2765    33.7804
  41  H    Isotropic =    26.3537   Anisotropy =     5.5380
XX=    25.2703   YX=     3.0665   ZX=    -1.1159
XY=     1.1276   YY=    27.5063   ZY=    -1.2352
XZ=     0.1939   YZ=    -3.2653   ZZ=    26.2844
Eigenvalues:    23.6687    25.3467    30.0457
  42  H    Isotropic =    26.3188   Anisotropy =     8.1778
XX=    24.9027   YX=     0.7174   ZX=     0.3536
XY=     3.3285   YY=    28.2549   ZY=    -5.9637
XZ=    -0.7422   YZ=    -2.2696   ZZ=    25.7987
Eigenvalues:    22.2523    24.9334    31.7706
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 52.11 | 69.59 | 85.61 | 98.93 | 125.11 | 152.41 |
| intensities | 1.33 | 2.60 | 0.02 | 3.09 | 1.76 | 7.30 |
| reduc. mass | 1.49 | 0.97 | 1.23 | 1.51 | 0.93 | 0.27 |
| force const | 0.00 | 0.00 | 0.01 | 0.01 | 0.01 | 0.00 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 173.97 | 191.72 | 225.59 | 246.52 | 251.59 | 257.65 |
| intensities | 2.48 | 2.98 | 1.27 | 0.56 | 2.68 | 3.70 |
| reduc. mass | 0.38 | 0.68 | 1.47 | 0.72 | 0.91 | 0.90 |
| force const | 0.01 | 0.01 | 0.04 | 0.03 | 0.03 | 0.04 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 275.93 | 302.06 | 303.83 | 315.30 | 327.71 | 332.02 |
| intensities | 1.27 | 0.46 | 5.40 | 1.74 | 0.29 | 6.24 |
| reduc. mass | 0.78 | 0.51 | 1.79 | 0.27 | 0.20 | 1.40 |
| force const | 0.04 | 0.03 | 0.10 | 0.02 | 0.01 | 0.09 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 364.94 | 397.73 | 425.93 | 459.89 | 485.43 | 501.00 |
| intensities | 0.51 | 3.10 | 13.15 | 1.57 | 3.21 | 13.93 |
| reduc. mass | 0.69 | 0.76 | 0.62 | 0.59 | 0.62 | 0.54 |
| force const | 0.05 | 0.07 | 0.07 | 0.07 | 0.09 | 0.08 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 521.13 | 534.04 | 547.45 | 554.70 | 568.37 | 598.84 |
| intensities | 19.50 | 13.92 | 10.59 | 19.25 | 66.84 | 20.28 |
| reduc. mass | 1.29 | 0.78 | 0.77 | 0.37 | 0.58 | 2.31 |
| force const | 0.21 | 0.13 | 0.14 | 0.07 | 0.11 | 0.49 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 654.74 | 667.72 | 696.09 | 712.75 | 716.96 | 743.08 |
| intensities | 83.73 | 30.85 | 4.48 | 13.11 | 0.92 | 0.92 |
| reduc. mass | 0.50 | 0.68 | 0.91 | 1.62 | 0.35 | 0.91 |
| force const | 0.13 | 0.18 | 0.26 | 0.49 | 0.11 | 0.29 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 750.20 | 803.05 | 832.33 | 847.59 | 869.13 | 922.47 |
| intensities | 7.22 | 2.84 | 2.80 | 1.90 | 7.41 | 1.18 |
| reduc. mass | 0.77 | 1.22 | 1.51 | 0.64 | 0.62 | 0.90 |
| force const | 0.26 | 0.46 | 0.62 | 0.27 | 0.28 | 0.45 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 933.71 | 936.66 | 958.30 | 1000.24 | 1006.69 | 1016.85 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 1.22 | 9.30 | 15.05 | 15.44 | 8.17 | 0.39 |
| reduc. mass | 0.79 | 0.59 | 0.28 | 0.25 | 0.28 | 0.24 |
| force const | 0.41 | 0.31 | 0.15 | 0.15 | 0.17 | 0.15 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1027.71 | 1046.84 | 1053.75 | 1058.48 | 1067.33 | 1095.47 |
| intensities | 24.21 | 35.21 | 8.58 | 5.36 | 13.47 | 36.53 |
| reduc. mass | 0.50 | 0.33 | 0.26 | 0.35 | 0.48 | 0.61 |
| force const | 0.31 | 0.21 | 0.17 | 0.23 | 0.32 | 0.43 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1106.90 | 1123.05 | 1131.11 | 1150.14 | 1164.86 | 1204.41 |
| intensities | 23.28 | 58.93 | 7.48 | 25.05 | 31.24 | 84.22 |
| reduc. mass | 0.54 | 0.50 | 0.40 | 0.51 | 0.57 | 0.56 |
| force const | 0.39 | 0.37 | 0.30 | 0.40 | 0.46 | 0.48 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1226.55 | 1245.26 | 1252.66 | 1270.64 | 1303.77 | 1342.02 |
| intensities | 19.99 | 38.93 | 80.64 | 21.24 | 30.36 | 10.42 |
| reduc. mass | 0.59 | 0.24 | 1.17 | 0.26 | 0.66 | 2.56 |
| force const | 0.52 | 0.22 | 1.08 | 0.25 | 0.66 | 2.72 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1352.29 | 1380.64 | 1401.82 | 1411.52 | 1435.67 | 1474.44 |
| intensities | 106.86 | 122.84 | 107.76 | 430.18 | 86.98 | 14.07 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.40 | 0.56 | 0.37 | 0.74 | 0.59 | 1.35 |
| force const | 0.43 | 0.62 | 0.42 | 0.87 | 0.71 | 1.72 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1500.20 | 1509.98 | 1513.16 | 1520.86 | 1532.64 | 1537.93 |
| intensities | 1.86 | 18.01 | 153.58 | 1.42 | 17.94 | 30.09 |
| reduc. mass | 0.91 | 2.27 | 1.55 | 2.89 | 0.78 | 0.56 |
| force const | 1.20 | 3.05 | 2.08 | 3.93 | 1.08 | 0.78 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1559.97 | 1578.66 | 1591.59 | 1632.17 | 1633.05 | 1641.43 |
| intensities | 119.84 | 29.13 | 15.75 | 3.19 | 116.12 | 15.13 |
| reduc. mass | 0.82 | 0.58 | 0.54 | 0.64 | 0.42 | 0.47 |
| force const | 1.18 | 0.85 | 0.80 | 1.00 | 0.67 | 0.75 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1650.87 | 1656.69 | 1659.67 | 1662.84 | 1664.57 | 1667.57 |
| intensities | 34.34 | 3.89 | 59.63 | 26.34 | 30.03 | 8.83 |
| reduc. mass | 0.96 | 0.13 | 0.21 | 0.18 | 0.22 | 0.21 |
| force const | 1.53 | 0.21 | 0.34 | 0.29 | 0.35 | 0.35 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1670.16 | 1672.56 | 1673.65 | 1683.65 | 1690.75 | 1802.06 |
| intensities | 13.71 | 15.40 | 16.24 | 61.34 | 29.03 | 856.47 |
| reduc. mass | 0.18 | 0.13 | 0.16 | 0.67 | 0.25 | 1.58 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 0.29 | 0.22 | 0.26 | 1.11 | 0.41 | 3.02 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1832.61 | 1888.87 | 3020.44 | 3024.28 | 3031.13 | 3051.04 |
| intensities | 387.23 | 16.69 | 297.03 | 407.43 | 718.53 | 649.94 |
| reduc. mass | 1.32 | 0.86 | 0.32 | 0.26 | 0.25 | 0.80 |
| force const | 2.62 | 1.81 | 1.75 | 1.38 | 1.35 | 4.37 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3056.27 | 3062.75 | 3076.07 | 3094.15 | 3102.37 | 3124.37 |
| intensities | 352.17 | 497.94 | 102.49 | 601.56 | 14.69 | 310.72 |
| reduc. mass | 0.32 | 0.34 | 0.81 | 0.38 | 0.69 | 0.53 |
| force const | 1.73 | 1.89 | 4.50 | 2.14 | 3.90 | 3.02 |

| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3128.34 | 3131.86 | 3133.95 | 3136.48 | 3145.81 | 3146.91 |
| intensities | 398.61 | 370.81 | 221.17 | 589.13 | 455.40 | 14.94 |
| reduc. mass | 0.36 | 0.34 | 0.44 | 0.45 | 0.32 | 0.30 |
| force const | 2.08 | 1.96 | 2.55 | 2.62 | 1.86 | 1.77 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3152.70 | 3155.05 | 3163.51 | 3195.69 | 3821.11 | 3849.77 |
| intensities | 513.75 | 361.51 | 287.95 | 318.53 | 100.44 | 88.02 |
| reduc. mass | 0.69 | 0.48 | 0.67 | 0.56 | 0.94 | 0.94 |
| force const | 4.04 | 2.81 | 3.96 | 3.37 | 8.13 | 8.25 |

Number of imaginary frequencies: 0

4. DFT calculation data for CBE with alternate configuration at C1 (**8**). Energies, optimized geometries, NMR shielding values and IR frequencies from calculations performed at the mPW1PW91/6-311+G(2d,p)//M06-2X-D3/6-31G(d,p) level.

Conformation 1

Boltzmann Population = 2.8% (relative energy = 1.71 kcal/mol)

Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.981775 hartrees

Total enthalpy, Htot (Utot + pV): -885.980831 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.043945 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.608400 | 1.672500 | 0.840200 |
| 2 | 6 | 0 | -3.419500 | 1.580600 | 2.363500 |
| 3 | 6 | 0 | -4.753100 | 1.313000 | 3.085100 |
| 4 | 6 | 0 | -5.642800 | 2.562000 | 2.900700 |
| 5 | 6 | 0 | -5.587100 | 3.122800 | 1.441200 |
| 6 | 6 | 0 | -5.006400 | 2.141900 | 0.413400 |
| 7 | 6 | 0 | -4.972500 | 2.773100 | -0.977100 |
| 8 | 6 | 0 | -4.506300 | 0.957200 | 4.537300 |
| 9 | 6 | 0 | -7.135600 | 2.409400 | 3.110000 |
| 10 | 6 | 0 | -7.793700 | 2.947600 | 2.007600 |
| 11 | 6 | 0 | -7.914500 | 1.951900 | 4.171100 |
| 12 | 6 | 0 | -9.309900 | 2.040800 | 4.086200 |
| 13 | 6 | 0 | -9.938100 | 2.574300 | 2.965500 |
| 14 | 6 | 0 | -9.167500 | 3.042600 | 1.894200 |
| 15 | 8 | 0 | -7.404300 | 1.452800 | 5.327900 |
| 16 | 8 | 0 | -6.941300 | 3.405400 | 1.041700 |
| 17 | 8 | 0 | -5.832600 | 0.982800 | 0.386100 |
| 18 | 6 | 0 | -11.442700 | 2.621200 | 2.879900 |
| 19 | 6 | 0 | -4.049600 | 2.044600 | 5.477900 |
| 20 | 6 | 0 | -4.683000 | -0.299200 | 4.961900 |
| 21 | 1 | 0 | -2.854000 | 2.340000 | 0.412100 |
| 22 | 1 | 0 | -3.469800 | 0.691300 | 0.376100 |
| 23 | 1 | 0 | -3.000000 | 2.521400 | 2.744000 |
| 24 | 1 | 0 | -2.698500 | 0.795400 | 2.608800 |
| 25 | 1 | 0 | -5.242900 | 0.465000 | 2.597800 |
| 26 | 1 | 0 | -5.258400 | 3.341500 | 3.572200 |
| 27 | 1 | 0 | -5.031600 | 4.066300 | 1.399200 |
| 28 | 1 | 0 | -4.344300 | 3.668600 | -0.992600 |
| 29 | 1 | 0 | -4.572500 | 2.049900 | -1.692600 |
| 30 | 1 | 0 | -5.981400 | 3.056800 | -1.288600 |
| 31 | 1 | 0 | -9.888600 | 1.672800 | 4.927000 |
| 32 | 1 | 0 | -9.620700 | 3.477200 | 1.010400 |
| 33 | 1 | 0 | -6.547100 | 1.030400 | 5.165600 |
| 34 | 1 | 0 | -6.732700 | 1.287100 | 0.204200 |
| 35 | 1 | 0 | -11.898800 | 2.545000 | 3.868900 |
| 36 | 1 | 0 | -11.781800 | 3.550600 | 2.414600 |
| 37 | 1 | 0 | -11.821700 | 1.793200 | 2.272000 |
| 38 | 1 | 0 | -3.698700 | 1.622000 | 6.421100 |
| 39 | 1 | 0 | -3.240500 | 2.639900 | 5.043200 |
| 40 | 1 | 0 | -4.874200 | 2.729900 | 5.703800 |
| 41 | 1 | 0 | -4.474200 | -0.587400 | 5.988100 |
| 42 | 1 | 0 | -5.032100 | -1.077100 | 4.289000 |

---

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 154.0790 Anisotropy = 27.4528

XX= 163.3952 YX= 12.8578 ZX= 0.8533

XY= 10.7070 YY= 156.9297 ZY= -0.6333

XZ= -3.3524 YZ= 3.4573 ZZ= 141.9122

Eigenvalues: 141.3734 148.4828 172.3809

2 C Isotropic = 156.8428 Anisotropy = 21.6747

```
XX=   169.7617   YX=    -4.4692   ZX=    -0.9102
XY=    -3.8113   YY=   159.4402   ZY=     4.6317
XZ=     1.7369   YZ=     6.4496   ZZ=   141.3265
Eigenvalues:   139.6875   159.5484   171.2926
   3  C    Isotropic =   138.6882   Anisotropy =    20.3035
XX=   135.0093   YX=     0.8482   ZX=    -0.0492
XY=     7.8516   YY=   150.2124   ZY=    -6.1279
XZ=     3.7277   YZ=    -3.5939   ZZ=   130.8428
Eigenvalues:   128.3893   135.4513   152.2238
   4  C    Isotropic =   138.4386   Anisotropy =    28.5966
XX=   157.2736   YX=     0.7062   ZX=     0.1092
XY=     1.1790   YY=   139.8651   ZY=     9.1683
XZ=    -6.0733   YZ=     9.7498   ZZ=   118.1772
Eigenvalues:   114.4039   143.4090   157.5030
   5  C    Isotropic =    98.7292   Anisotropy =    60.3174
XX=   129.7540   YX=    15.2255   ZX=     2.5697
XY=    21.3698   YY=   102.4928   ZY=    -0.6373
XZ=     1.2181   YZ=    -5.8264   ZZ=    63.9407
Eigenvalues:    63.4716    93.7751   138.9408
   6  C    Isotropic =   113.6232   Anisotropy =    45.9270
XX=   103.4586   YX=    -5.1170   ZX=   -19.5260
XY=    -2.1416   YY=   101.9861   ZY=     3.5515
XZ=   -14.4617   YZ=    10.4834   ZZ=   135.4249
Eigenvalues:    96.0476   100.5807   144.2412
   7  C    Isotropic =   158.0045   Anisotropy =    44.6531
XX=   141.1154   YX=    -4.7063   ZX=   -10.2472
XY=    -5.4945   YY=   183.9261   ZY=    13.8076
XZ=   -10.3514   YZ=     5.8643   ZZ=   148.9720
Eigenvalues:   133.9779   152.2624   187.7732
   8  C    Isotropic =    23.6043   Anisotropy =   200.3924
XX=   154.8070   YX=   -15.3655   ZX=    21.1269
XY=   -14.9763   YY=   -51.7867   ZY=    57.7618
XZ=    16.9147   YZ=    52.2818   ZZ=   -32.2075
Eigenvalues:  -100.1151    13.7287   157.1992
   9  C    Isotropic =    70.7856   Anisotropy =   104.5327
XX=    26.2159   YX=     6.4872   ZX=    28.5761
XY=   -17.7372   YY=    53.3032   ZY=    -7.5662
XZ=    27.7809   YZ=    -5.1108   ZZ=   132.8377
Eigenvalues:    18.7727    53.1101   140.4741
  10  C    Isotropic =    20.0350   Anisotropy =   103.9133
XX=     1.7390   YX=    33.8978   ZX=    24.2250
XY=    45.1701   YY=   -20.0146   ZY=   -26.9214
XZ=    32.8012   YZ=   -23.3645   ZZ=    78.3807
Eigenvalues:   -60.2125    31.0071    89.3105
  11  C    Isotropic =    27.0503   Anisotropy =   131.8422
XX=    11.1027   YX=   -30.6612   ZX=    13.8879
XY=   -22.2181   YY=   -39.8880   ZY=   -17.0900
XZ=    19.3579   YZ=   -11.7401   ZZ=   109.9363
Eigenvalues:   -51.4169    17.6228   114.9451
  12  C    Isotropic =    71.6213   Anisotropy =   114.7213
XX=    49.1917   YX=    31.8198   ZX=    22.5962
XY=    38.2350   YY=    27.6019   ZY=   -23.4577
```

```
XZ=    35.5996   YZ=   -22.3768   ZZ=   138.0703
Eigenvalues:    -7.1155    73.8772   148.1021
  13  C    Isotropic =    40.9933   Anisotropy =   193.8321
XX=   -47.3437   YX=   -12.5454   ZX=    41.7926
XY=   -17.4028   YY=    10.0440   ZY=   -17.9439
XZ=    35.3226   YZ=   -21.1819   ZZ=   160.2797
Eigenvalues:   -56.2555     9.0208   170.2148
  14  C    Isotropic =    82.7465   Anisotropy =   118.9064
XX=    74.4883   YX=   -18.1086   ZX=    15.4016
XY=   -30.8208   YY=    18.9770   ZY=   -15.2620
XZ=    19.4944   YZ=   -20.2757   ZZ=   154.7742
Eigenvalues:     8.9476    77.2745   162.0175
  15  O    Isotropic =   206.0643   Anisotropy =    57.3019
XX=   165.8279   YX=    14.6266   ZX=     5.8961
XY=     8.6664   YY=   216.2362   ZY=     4.6526
XZ=    42.6696   YZ=   -19.9348   ZZ=   236.1288
Eigenvalues:   155.3040   218.6234   244.2656
  16  O    Isotropic =   193.4394   Anisotropy =   109.8629
XX=   178.4785   YX=   -66.7719   ZX=    -9.1045
XY=   -46.8013   YY=   228.9565   ZY=    14.1094
XZ=     4.2324   YZ=     3.6492   ZZ=   172.8832
Eigenvalues:   141.3221   172.3148   266.6814
  17  O    Isotropic =   259.2172   Anisotropy =    45.4693
XX=   281.5546   YX=    13.6274   ZX=   -25.9226
XY=     3.6313   YY=   251.1307   ZY=    27.7233
XZ=   -11.7212   YZ=     8.9034   ZZ=   244.9663
Eigenvalues:   222.6441   265.4774   289.5301
  18  C    Isotropic =   164.1706   Anisotropy =    40.9509
XX=   189.8082   YX=     2.5234   ZX=    -3.8524
XY=     6.5458   YY=   157.3424   ZY=     1.5525
XZ=   -10.4270   YZ=     0.7026   ZZ=   145.3611
Eigenvalues:   143.9879   157.0526   191.4712
  19  C    Isotropic =   167.3127   Anisotropy =    24.5941
XX=   160.5528   YX=     3.9665   ZX=    -2.6628
XY=     2.9899   YY=   164.9931   ZY=   -13.4835
XZ=    -4.0707   YZ=    -7.7946   ZZ=   176.3922
Eigenvalues:   157.7894   160.4400   183.7087
  20  C    Isotropic =    66.9907   Anisotropy =   112.5905
XX=   140.9087   YX=    -7.9911   ZX=     7.2026
XY=   -10.4157   YY=     5.0193   ZY=    58.5436
XZ=    12.0676   YZ=    58.6934   ZZ=    55.0441
Eigenvalues:   -34.6616    93.5826   142.0511
  21  H    Isotropic =    30.2160   Anisotropy =     8.5384
XX=    32.6953   YX=    -2.4374   ZX=    -3.5458
XY=    -1.9606   YY=    31.7635   ZY=     1.2121
XZ=    -4.0762   YZ=     0.9800   ZZ=    26.1891
Eigenvalues:    24.4308    30.3090    35.9082
  22  H    Isotropic =    29.8417   Anisotropy =     7.7572
XX=    30.4312   YX=    -0.2725   ZX=     4.5965
XY=     0.2339   YY=    29.0522   ZY=    -1.9023
XZ=     4.3106   YZ=    -1.9749   ZZ=    30.0417
Eigenvalues:    25.2459    29.2659    35.0131
```

```
  23  H    Isotropic =    30.1850   Anisotropy =     6.7787
XX=    29.8385   YX=    -0.4198   ZX=    -4.4750
XY=    -0.5835   YY=    30.4923   ZY=    -2.4294
XZ=    -3.6335   YZ=    -2.6884   ZZ=    30.2241
Eigenvalues:    25.0921    30.7587    34.7041
  24  H    Isotropic =    30.3571   Anisotropy =     9.0000
XX=    33.5877   YX=     2.2937   ZX=     3.4102
XY=     2.6986   YY=    31.5017   ZY=     1.1566
XZ=     3.4806   YZ=     0.5988   ZZ=    25.9819
Eigenvalues:    24.6522    30.0620    36.3571
  25  H    Isotropic =    27.9996   Anisotropy =     5.1465
XX=    24.6851   YX=     0.1542   ZX=    -1.3096
XY=    -0.4134   YY=    31.3100   ZY=    -0.5403
XZ=     0.2924   YZ=     1.7859   ZZ=    28.0036
Eigenvalues:    24.6087    27.9594    31.4306
  26  H    Isotropic =    27.8675   Anisotropy =     6.4460
XX=    25.4027   YX=     1.5470   ZX=     0.5560
XY=     1.0177   YY=    29.8237   ZY=    -1.9151
XZ=    -2.4186   YZ=    -3.2739   ZZ=    28.3762
Eigenvalues:    25.0306    26.4072    32.1649
  27  H    Isotropic =    27.2232   Anisotropy =     4.0658
XX=    25.9630   YX=     0.3590   ZX=    -2.0248
XY=     0.5130   YY=    26.9113   ZY=     1.3088
XZ=    -1.2093   YZ=     1.4361   ZZ=    28.7952
Eigenvalues:    24.7470    26.9889    29.9337
  28  H    Isotropic =    30.9757   Anisotropy =    10.2540
XX=    29.0320   YX=    -2.2461   ZX=    -3.0318
XY=    -2.8063   YY=    32.1664   ZY=     4.7629
XZ=    -2.9464   YZ=     3.4995   ZZ=    31.7288
Eigenvalues:    27.0917    28.0237    37.8117
  29  H    Isotropic =    30.5456   Anisotropy =     8.6827
XX=    29.3342   YX=    -2.3951   ZX=     2.0885
XY=    -3.1817   YY=    33.5123   ZY=    -3.0053
XZ=     2.4230   YZ=    -2.0278   ZZ=    28.7904
Eigenvalues:    26.7899    28.5129    36.3341
  30  H    Isotropic =    30.1997   Anisotropy =     7.7787
XX=    31.0557   YX=     1.1384   ZX=     0.7436
XY=     2.8024   YY=    34.4753   ZY=     0.1841
XZ=     0.7364   YZ=    -0.1151   ZZ=    25.0681
Eigenvalues:    24.9733    30.2402    35.3855
  31  H    Isotropic =    25.3284   Anisotropy =     7.0635
XX=    28.4814   YX=     2.3898   ZX=    -0.7681
XY=     2.4469   YY=    25.9780   ZY=     0.0608
XZ=    -1.0054   YZ=    -0.4086   ZZ=    21.5259
Eigenvalues:    21.4102    24.5376    30.0374
  32  H    Isotropic =    25.4158   Anisotropy =     7.3190
XX=    30.0108   YX=    -0.7606   ZX=    -1.2223
XY=    -0.4581   YY=    24.6005   ZY=     0.6877
XZ=    -1.3251   YZ=     1.0562   ZZ=    21.6361
Eigenvalues:    21.2644    24.6879    30.2952
  33  H    Isotropic =    25.6723   Anisotropy =    23.8263
XX=    40.1447   YX=     1.4051   ZX=     4.0388
```

```
XY=     2.6778   YY=    21.8583   ZY=     2.2557
XZ=     6.4526   YZ=     4.3103   ZZ=    15.0140
Eigenvalues:    13.0367    22.4238    41.5566
  34  H    Isotropic =    30.5153   Anisotropy =    15.0221
XX=    38.5892   YX=     5.3537   ZX=    -0.7781
XY=     5.0802   YY=    24.7849   ZY=    -2.6696
XZ=    -0.6340   YZ=    -2.6652   ZZ=    28.1718
Eigenvalues:    22.1364    28.8795    40.5301
  35  H    Isotropic =    29.8117   Anisotropy =     8.0012
XX=    33.4891   YX=    -3.7325   ZX=    -0.3059
XY=    -1.3585   YY=    31.2335   ZY=    -0.3855
XZ=     0.1766   YZ=    -0.0738   ZZ=    24.7127
Eigenvalues:    24.7016    29.5878    35.1459
  36  H    Isotropic =    29.5899   Anisotropy =     8.1707
XX=    32.2024   YX=     3.4046   ZX=     1.7471
XY=     1.4004   YY=    29.6936   ZY=     3.2978
XZ=     1.7535   YZ=     3.4146   ZZ=    26.8736
Eigenvalues:    24.6406    29.0920    35.0370
  37  H    Isotropic =    29.3677   Anisotropy =     8.6934
XX=    29.7957   YX=     1.3303   ZX=    -3.2045
XY=     1.1298   YY=    27.3263   ZY=    -2.2166
XZ=    -4.3877   YZ=    -2.7708   ZZ=    30.9811
Eigenvalues:    25.8165    27.1233    35.1633
  38  H    Isotropic =    29.8899   Anisotropy =     8.7679
XX=    26.8507   YX=     2.7206   ZX=    -0.6715
XY=     2.2359   YY=    34.8213   ZY=    -0.1810
XZ=    -0.8015   YZ=    -2.0224   ZZ=    27.9976
Eigenvalues:    26.0505    27.8840    35.7352
  39  H    Isotropic =    29.9424   Anisotropy =     6.6647
XX=    29.4652   YX=    -1.1384   ZX=    -4.6742
XY=    -0.6049   YY=    30.3939   ZY=    -2.0605
XZ=    -4.5828   YZ=    -0.5671   ZZ=    29.9680
Eigenvalues:    24.6681    30.7735    34.3855
  40  H    Isotropic =    29.4652   Anisotropy =     5.4008
XX=    30.7600   YX=     0.5158   ZX=     3.2155
XY=     0.4042   YY=    28.5560   ZY=    -2.6037
XZ=     2.1944   YZ=    -2.2657   ZZ=    29.0795
Eigenvalues:    25.4156    29.9142    33.0657
  41  H    Isotropic =    26.4705   Anisotropy =     6.5098
XX=    25.4168   YX=     0.7190   ZX=     0.3148
XY=     0.6274   YY=    26.8573   ZY=     2.0187
XZ=     0.6352   YZ=     5.3591   ZZ=    27.1376
Eigenvalues:    23.2940    25.3072    30.8104
  42  H    Isotropic =    26.2690   Anisotropy =     7.2958
XX=    25.3149   YX=     0.2203   ZX=     0.3926
XY=    -0.2831   YY=    25.9681   ZY=     5.7083
XZ=     1.0409   YZ=     2.8276   ZZ=    27.5240
Eigenvalues:    22.3287    25.3454    31.1329
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 53.56 | 64.57 | 84.42 | 98.42 | 118.11 | 136.08 |
| intensities | 0.70 | 1.09 | 0.32 | 1.03 | 1.06 | 5.40 |
| reduc. mass | 1.30 | 1.48 | 0.84 | 1.55 | 0.27 | 1.68 |
| force const | 0.00 | 0.00 | 0.00 | 0.01 | 0.00 | 0.02 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 155.89 | 193.48 | 211.26 | 230.85 | 235.29 | 257.81 |
| intensities | 1.05 | 5.04 | 1.20 | 4.21 | 2.50 | 0.58 |
| reduc. mass | 0.74 | 0.66 | 0.61 | 0.39 | 1.31 | 2.29 |
| force const | 0.01 | 0.01 | 0.02 | 0.01 | 0.04 | 0.09 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 269.40 | 284.98 | 292.63 | 306.06 | 316.19 | 338.73 |
| intensities | 0.52 | 0.46 | 1.85 | 0.76 | 0.09 | 2.23 |
| reduc. mass | 0.69 | 0.48 | 0.43 | 0.38 | 2.98 | 0.84 |
| force const | 0.03 | 0.02 | 0.02 | 0.02 | 0.18 | 0.06 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 360.13 | 392.41 | 396.11 | 446.07 | 470.25 | 499.72 |
| intensities | 4.19 | 1.80 | 4.52 | 1.85 | 0.04 | 15.72 |
| reduc. mass | 0.67 | 0.69 | 1.69 | 1.19 | 0.63 | 0.56 |
| force const | 0.05 | 0.06 | 0.16 | 0.14 | 0.08 | 0.08 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 521.63 | 529.47 | 536.48 | 553.56 | 574.61 | 592.07 |
| intensities | 7.57 | 22.07 | 16.17 | 2.90 | 124.46 | 6.61 |
| reduc. mass | 0.53 | 1.42 | 0.40 | 0.86 | 0.50 | 0.37 |
| force const | 0.09 | 0.23 | 0.07 | 0.16 | 0.10 | 0.08 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 610.70 | 669.11 | 685.63 | 710.07 | 725.31 | 732.80 |
| intensities | 119.60 | 0.91 | 4.61 | 3.01 | 1.17 | 0.60 |
| reduc. mass | 0.55 | 0.85 | 1.25 | 0.33 | 0.87 | 0.70 |
| force const | 0.12 | 0.22 | 0.35 | 0.10 | 0.27 | 0.22 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 745.32 | 772.77 | 794.58 | 827.61 | 852.11 | 902.78 |
| intensities | 2.42 | 1.63 | 6.17 | 15.76 | 11.02 | 1.79 |
| reduc. mass | 0.99 | 0.36 | 2.42 | 1.17 | 0.63 | 0.59 |
| force const | 0.32 | 0.13 | 0.90 | 0.47 | 0.27 | 0.28 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 932.17 | 937.85 | 949.88 | 993.78 | 1003.80 | 1021.20 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 5.36 | 1.18 | 15.18 | 3.81 | 8.46 | 11.88 |
| reduc. mass | 0.46 | 0.58 | 0.63 | 0.30 | 0.26 | 0.21 |
| force const | 0.24 | 0.30 | 0.33 | 0.17 | 0.15 | 0.13 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1028.88 | 1032.98 | 1038.20 | 1063.42 | 1065.98 | 1093.60 |
| intensities | 14.76 | 7.74 | 5.90 | 18.03 | 43.53 | 6.55 |
| reduc. mass | 0.27 | 0.27 | 0.32 | 0.33 | 0.30 | 0.68 |
| force const | 0.17 | 0.17 | 0.20 | 0.22 | 0.20 | 0.48 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1097.55 | 1126.47 | 1130.14 | 1143.24 | 1158.15 | 1207.08 |
| intensities | 80.78 | 90.47 | 13.17 | 45.74 | 18.23 | 136.51 |
| reduc. mass | 0.71 | 0.75 | 0.62 | 0.62 | 0.25 | 1.66 |
| force const | 0.51 | 0.56 | 0.46 | 0.48 | 0.20 | 1.42 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1227.04 | 1245.76 | 1256.65 | 1264.64 | 1299.16 | 1344.45 |
| intensities | 48.08 | 43.48 | 114.86 | 10.31 | 64.92 | 21.93 |
| reduc. mass | 0.75 | 0.33 | 0.98 | 0.29 | 1.04 | 0.43 |
| force const | 0.66 | 0.30 | 0.92 | 0.27 | 1.03 | 0.46 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1377.12 | 1383.81 | 1389.86 | 1411.21 | 1443.66 | 1451.61 |
| intensities | 33.99 | 397.98 | 41.56 | 40.97 | 65.35 | 48.79 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.40 | 0.80 | 0.74 | 1.01 | 3.06 | 0.81 |
| force const | 0.45 | 0.90 | 0.84 | 1.18 | 3.76 | 1.01 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1491.03 | 1494.42 | 1503.62 | 1522.45 | 1528.92 | 1553.00 |
| intensities | 73.37 | 15.20 | 1.00 | 242.30 | 10.82 | 5.73 |
| reduc. mass | 0.52 | 0.66 | 0.58 | 0.93 | 0.77 | 0.53 |
| force const | 0.67 | 0.87 | 0.77 | 1.27 | 1.06 | 0.76 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1562.86 | 1577.44 | 1589.74 | 1616.44 | 1631.12 | 1638.93 |
| intensities | 58.20 | 24.77 | 63.41 | 143.45 | 17.32 | 18.21 |
| reduc. mass | 0.53 | 0.70 | 0.44 | 0.60 | 0.45 | 0.16 |
| force const | 0.76 | 1.02 | 0.66 | 0.92 | 0.70 | 0.25 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1643.36 | 1646.92 | 1653.68 | 1659.53 | 1661.89 | 1663.06 |
| intensities | 33.86 | 3.07 | 31.05 | 18.30 | 26.49 | 17.29 |
| reduc. mass | 0.14 | 0.26 | 0.20 | 0.37 | 0.12 | 0.28 |
| force const | 0.23 | 0.41 | 0.33 | 0.60 | 0.20 | 0.45 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1664.69 | 1667.70 | 1670.57 | 1676.64 | 1706.42 | 1790.81 |
| intensities | 16.59 | 47.86 | 16.94 | 99.83 | 173.08 | 808.37 |
| reduc. mass | 0.28 | 0.15 | 0.14 | 0.27 | 0.64 | 1.44 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 0.45 | 0.25 | 0.24 | 0.44 | 1.10 | 2.72 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1849.12 | 1890.38 | 3011.79 | 3026.43 | 3030.60 | 3055.53 |
| intensities | 400.64 | 18.58 | 702.54 | 390.78 | 626.70 | 371.69 |
| reduc. mass | 1.57 | 0.86 | 0.24 | 0.27 | 0.25 | 0.45 |
| force const | 3.17 | 1.81 | 1.29 | 1.47 | 1.33 | 2.47 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3056.63 | 3079.66 | 3090.41 | 3094.83 | 3102.86 | 3120.54 |
| intensities | 388.07 | 295.97 | 672.94 | 389.92 | 55.83 | 516.38 |
| reduc. mass | 0.28 | 0.51 | 0.42 | 0.86 | 0.46 | 0.13 |
| force const | 1.52 | 2.85 | 2.37 | 4.87 | 2.63 | 0.72 |

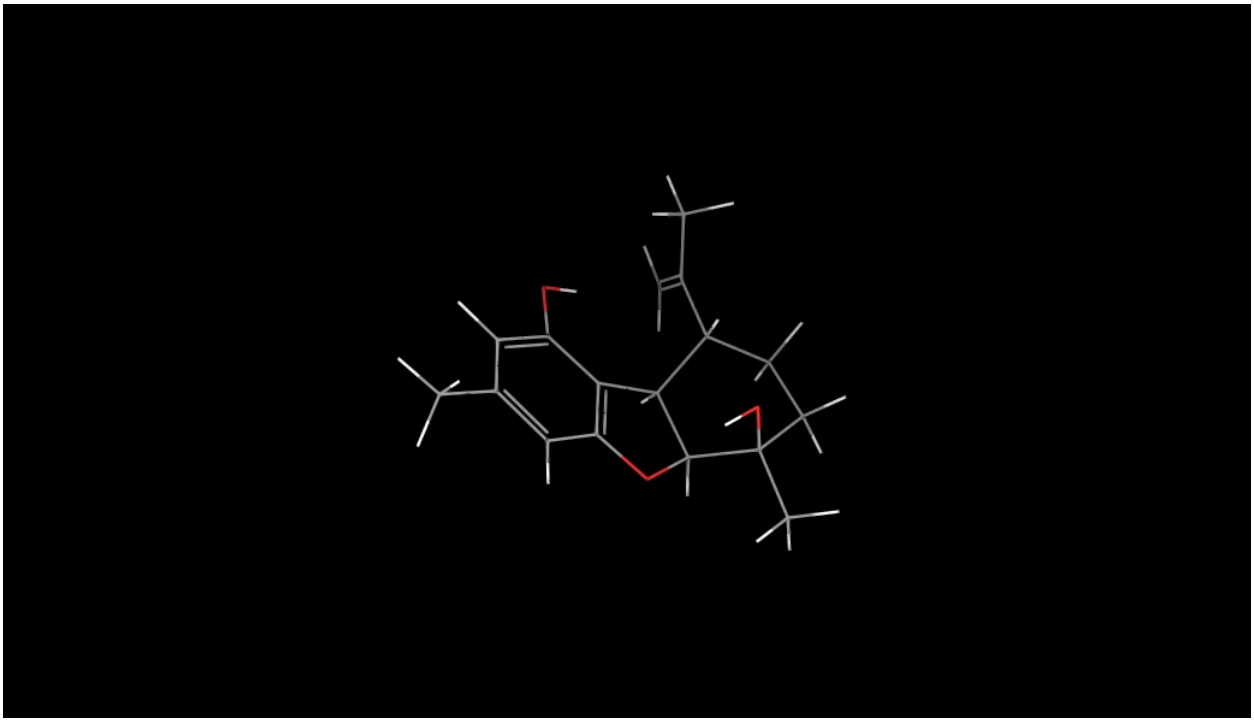
| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3126.44 | 3132.77 | 3138.04 | 3141.65 | 3146.01 | 3146.92 |
| intensities | 317.26 | 210.53 | 447.04 | 443.01 | 208.44 | 509.93 |
| reduc. mass | 0.30 | 0.16 | 0.23 | 0.51 | 0.23 | 0.19 |
| force const | 1.72 | 0.95 | 1.34 | 2.98 | 1.36 | 1.10 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3147.52 | 3160.68 | 3180.92 | 3197.16 | 3829.28 | 3835.72 |
| intensities | 205.94 | 179.13 | 389.86 | 373.33 | 63.84 | 438.19 |
| reduc. mass | 0.23 | 0.47 | 0.62 | 0.55 | 0.92 | 0.92 |
| force const | 1.34 | 2.78 | 3.71 | 3.34 | 7.92 | 7.94 |

Number of imaginary frequencies: 0

Conformation 2

Boltzmann Population = 9.1% (relative energy = 1.01 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.982115 hartrees

Total enthalpy, Htot (Utot + pV): -885.981170 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.043739 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.540900 | 1.828700 | 0.862200 |
| 2 | 6 | 0 | -3.423200 | 1.594900 | 2.380100 |
| 3 | 6 | 0 | -4.783600 | 1.359900 | 3.058900 |
| 4 | 6 | 0 | -5.644300 | 2.630000 | 2.874100 |
| 5 | 6 | 0 | -5.637400 | 3.147900 | 1.397600 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 6 | 0 | -4.945900 | 2.216100 | 0.389400 |
| 7 | 6 | 0 | -4.896000 | 2.870500 | -0.990900 |
| 8 | 6 | 0 | -4.578500 | 0.977300 | 4.515400 |
| 9 | 6 | 0 | -7.127700 | 2.479800 | 3.134800 |
| 10 | 6 | 0 | -7.826800 | 2.851700 | 1.989600 |
| 11 | 6 | 0 | -7.865400 | 2.090300 | 4.250200 |
| 12 | 6 | 0 | -9.264100 | 2.043500 | 4.165400 |
| 13 | 6 | 0 | -9.931000 | 2.394900 | 2.997600 |
| 14 | 6 | 0 | -9.202900 | 2.819400 | 1.877800 |
| 15 | 8 | 0 | -7.317000 | 1.747300 | 5.440900 |
| 16 | 8 | 0 | -7.010700 | 3.263400 | 0.973700 |
| 17 | 8 | 0 | -5.692100 | 1.007800 | 0.310700 |
| 18 | 6 | 0 | -11.434900 | 2.317400 | 2.919900 |
| 19 | 6 | 0 | -4.966900 | -0.430400 | 4.874000 |
| 20 | 6 | 0 | -4.067800 | 1.825200 | 5.415900 |
| 21 | 1 | 0 | -2.832400 | 2.602300 | 0.549400 |
| 22 | 1 | 0 | -3.284400 | 0.920400 | 0.308800 |
| 23 | 1 | 0 | -2.961800 | 2.466000 | 2.862500 |
| 24 | 1 | 0 | -2.758800 | 0.749800 | 2.584200 |
| 25 | 1 | 0 | -5.291700 | 0.536300 | 2.550100 |
| 26 | 1 | 0 | -5.215300 | 3.411100 | 3.516000 |
| 27 | 1 | 0 | -5.192100 | 4.147400 | 1.336600 |
| 28 | 1 | 0 | -5.907700 | 3.102100 | -1.335400 |
| 29 | 1 | 0 | -4.318900 | 3.799600 | -0.971500 |
| 30 | 1 | 0 | -4.431600 | 2.181800 | -1.701600 |
| 31 | 1 | 0 | -9.812400 | 1.731100 | 5.047700 |
| 32 | 1 | 0 | -9.691600 | 3.122600 | 0.958900 |
| 33 | 1 | 0 | -6.357800 | 1.889300 | 5.423700 |
| 34 | 1 | 0 | -6.606200 | 1.263800 | 0.123700 |
| 35 | 1 | 0 | -11.876600 | 2.163600 | 3.906300 |
| 36 | 1 | 0 | -11.853100 | 3.234500 | 2.495500 |
| 37 | 1 | 0 | -11.747300 | 1.488100 | 2.277300 |
| 38 | 1 | 0 | -4.750200 | -0.662400 | 5.918900 |
| 39 | 1 | 0 | -6.038100 | -0.576500 | 4.696500 |
| 40 | 1 | 0 | -4.432800 | -1.142900 | 4.235700 |
| 41 | 1 | 0 | -3.902100 | 1.521000 | 6.445000 |
| 42 | 1 | 0 | -3.779400 | 2.839900 | 5.154600 |

---

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 154.4490 Anisotropy = 27.8000
XX= 160.2047 YX= 11.8359 ZX= -0.5956
XY= 10.3046 YY= 163.0871 ZY= -2.9653
XZ= -4.1687 YZ= 0.8048 ZZ= 140.0553
Eigenvalues: 139.7750 150.5897 172.9824

2 C Isotropic = 155.0107 Anisotropy = 24.7051
XX= 163.3269 YX= -9.5085 ZX= -6.2974
XY= -8.0240 YY= 161.8931 ZY= -8.0747
XZ= -4.6718 YZ= -7.9924 ZZ= 139.8123
Eigenvalues: 134.8687 158.6827 171.4808

3 C Isotropic = 143.1577 Anisotropy = 15.2162

```
XX=   143.0217   YX=    -1.2975   ZX=     3.1882
XY=     5.8050   YY=   152.8052   ZY=    -1.7601
XZ=     3.2847   YZ=    -0.0837   ZZ=   133.6461
Eigenvalues:   132.5170   143.6542   153.3018
   4  C    Isotropic =   133.7347   Anisotropy =    23.7195
XX=   143.3683   YX=     7.9786   ZX=     3.2446
XY=     3.6982   YY=   141.4159   ZY=     5.2901
XZ=     2.2954   YZ=     7.7406   ZZ=   116.4200
Eigenvalues:   114.7614   136.8951   149.5477
   5  C    Isotropic =    98.1095   Anisotropy =    59.5781
XX=   125.4409   YX=    16.3623   ZX=    -2.0251
XY=    22.5673   YY=   105.1827   ZY=    -6.3306
XZ=    -4.4454   YZ=    -8.0698   ZZ=    63.7048
Eigenvalues:    62.4904    94.0099   137.8282
   6  C    Isotropic =   114.2915   Anisotropy =    47.2893
XX=   102.6099   YX=    -4.6687   ZX=   -19.0953
XY=    -1.3402   YY=   102.2769   ZY=     1.5098
XZ=   -15.2842   YZ=     9.2072   ZZ=   137.9877
Eigenvalues:    95.5347   101.5221   145.8177
   7  C    Isotropic =   157.6235   Anisotropy =    45.8687
XX=   139.6956   YX=   -10.5963   ZX=   -10.6192
XY=   -11.2049   YY=   182.4203   ZY=    12.3477
XZ=    -8.8675   YZ=     5.0250   ZZ=   150.7547
Eigenvalues:   133.4105   151.2575   188.2027
   8  C    Isotropic =    16.0275   Anisotropy =   213.2761
XX=   146.1139   YX=    29.5610   ZX=    45.5258
XY=    27.3201   YY=   -64.5882   ZY=   -52.7544
XZ=    45.2269   YZ=   -44.9127   ZZ=   -33.4431
Eigenvalues:  -110.0620    -0.0670   158.2116
   9  C    Isotropic =    72.8771   Anisotropy =    98.8261
XX=    29.9773   YX=     7.7864   ZX=    26.0988
XY=   -16.2151   YY=    56.3515   ZY=     5.1772
XZ=    26.0041   YZ=     5.3441   ZZ=   132.3027
Eigenvalues:    22.8756    56.9946   138.7612
  10  C    Isotropic =    20.4887   Anisotropy =   103.8632
XX=    -4.8876   YX=    37.7034   ZX=    24.6767
XY=    50.7268   YY=   -16.7547   ZY=   -12.6131
XZ=    25.3873   YZ=   -10.8805   ZZ=    83.1085
Eigenvalues:   -59.9563    31.6916    89.7309
  11  C    Isotropic =    27.0468   Anisotropy =   135.2719
XX=    15.4562   YX=   -22.0826   ZX=    25.3061
XY=   -11.7114   YY=   -43.5828   ZY=     9.5603
XZ=    31.1709   YZ=     8.7327   ZZ=   109.2670
Eigenvalues:   -49.8023    13.7147   117.2281
  12  C    Isotropic =    73.7269   Anisotropy =   111.9335
XX=    44.5996   YX=    36.5475   ZX=    24.1900
XY=    43.1442   YY=    34.4336   ZY=    -7.2065
XZ=    25.7848   YZ=    -3.4761   ZZ=   142.1475
Eigenvalues:    -3.5980    76.4295   148.3492
  13  C    Isotropic =    40.9227   Anisotropy =   193.7961
XX=   -41.4369   YX=   -10.7128   ZX=    51.4203
XY=   -17.4672   YY=     5.4996   ZY=     6.6959
```

```
XZ=    46.5775   YZ=     6.4112   ZZ=   158.7052
Eigenvalues:   -56.5197     9.1676   170.1200
  14  C    Isotropic =    83.8167   Anisotropy =   118.9230
XX=    80.1620   YX=    -9.4564   ZX=    20.8652
XY=   -22.1534   YY=    14.3996   ZY=     5.9205
XZ=    24.5160   YZ=     1.5709   ZZ=   156.8884
Eigenvalues:    10.2603    78.0910   163.0986
  15  O    Isotropic =   191.6540   Anisotropy =    75.3659
XX=   155.9419   YX=    17.5521   ZX=    24.1227
XY=    11.4829   YY=   191.2402   ZY=   -11.1961
XZ=    29.2958   YZ=   -31.3219   ZZ=   227.7798
Eigenvalues:   138.7283   194.3358   241.8979
  16  O    Isotropic =   190.6984   Anisotropy =   108.9576
XX=   188.6211   YX=   -71.4905   ZX=     0.3752
XY=   -47.1951   YY=   216.1973   ZY=    10.1196
XZ=     9.4039   YZ=    -3.9529   ZZ=   167.2769
Eigenvalues:   140.2631   168.4953   263.3368
  17  O    Isotropic =   259.6782   Anisotropy =    39.8128
XX=   275.4369   YX=    13.1940   ZX=   -25.2377
XY=     4.7430   YY=   254.6246   ZY=    25.9279
XZ=   -14.7561   YZ=     3.3624   ZZ=   248.9731
Eigenvalues:   227.4158   265.3987   286.2200
  18  C    Isotropic =   164.0796   Anisotropy =    41.2270
XX=   188.3055   YX=     3.3993   ZX=    -7.5796
XY=     7.9143   YY=   157.8369   ZY=    -1.2256
XZ=   -12.5552   YZ=    -0.8908   ZZ=   146.0965
Eigenvalues:   143.8148   156.8598   191.5643
  19  C    Isotropic =   158.7158   Anisotropy =    41.4672
XX=   140.8536   YX=    -4.6584   ZX=    -7.1747
XY=    -3.2093   YY=   166.3408   ZY=    15.3256
XZ=    -7.4310   YZ=    19.1616   ZZ=   168.9531
Eigenvalues:   139.0647   150.7222   186.3606
  20  C    Isotropic =    72.6775   Anisotropy =   133.9116
XX=   155.4085   YX=    27.3810   ZX=    21.4245
XY=    26.3611   YY=    -7.0488   ZY=   -47.4011
XZ=    20.7367   YZ=   -50.1306   ZZ=    69.6729
Eigenvalues:   -36.5506    92.6312   161.9519
  21  H    Isotropic =    30.2315   Anisotropy =     8.4234
XX=    32.4112   YX=    -1.9569   ZX=    -4.3785
XY=    -1.5308   YY=    31.1945   ZY=     1.0926
XZ=    -4.8130   YZ=     0.5154   ZZ=    27.0887
Eigenvalues:    24.4345    30.4128    35.8471
  22  H    Isotropic =    29.8620   Anisotropy =     7.8656
XX=    30.9974   YX=    -0.5421   ZX=     4.7553
XY=    -0.1299   YY=    29.5930   ZY=    -1.6389
XZ=     4.6689   YZ=    -1.5251   ZZ=    28.9957
Eigenvalues:    24.9483    29.5320    35.1058
  23  H    Isotropic =    30.4936   Anisotropy =     7.3982
XX=    30.3319   YX=    -0.1204   ZX=    -4.2048
XY=    -0.0009   YY=    30.9382   ZY=    -3.5604
XZ=    -3.3122   YZ=    -3.1491   ZZ=    30.2107
Eigenvalues:    25.3272    30.7278    35.4257
```

```
  24  H    Isotropic =    30.0627   Anisotropy =     8.4377
XX=    32.6136   YX=     1.4893   ZX=     3.4176
XY=     2.4847   YY=    31.5559   ZY=     2.2891
XZ=     3.4668   YZ=     1.3998   ZZ=    26.0186
Eigenvalues:    24.4194    30.0809    35.6878
  25  H    Isotropic =    28.5521   Anisotropy =     6.0672
XX=    24.7610   YX=    -0.9956   ZX=    -1.4109
XY=    -1.0798   YY=    32.2709   ZY=    -0.1167
XZ=     0.1320   YZ=     1.6673   ZZ=    28.6245
Eigenvalues:    24.5499    28.5096    32.5969
  26  H    Isotropic =    28.1742   Anisotropy =     5.5668
XX=    25.8213   YX=     1.0890   ZX=     0.2336
XY=    -0.1932   YY=    29.0548   ZY=    -1.8062
XZ=    -2.1684   YZ=    -2.8807   ZZ=    29.6464
Eigenvalues:    25.5851    27.0520    31.8854
  27  H    Isotropic =    27.0581   Anisotropy =     4.3754
XX=    25.4798   YX=     0.1361   ZX=    -2.0824
XY=    -0.0620   YY=    27.0002   ZY=     1.0972
XZ=    -1.5938   YZ=     1.4419   ZZ=    28.6945
Eigenvalues:    24.5058    26.6936    29.9751
  28  H    Isotropic =    30.1616   Anisotropy =     7.8732
XX=    30.5075   YX=     0.6188   ZX=     0.3846
XY=     2.3474   YY=    34.9594   ZY=     0.0811
XZ=     0.3855   YZ=    -0.0046   ZZ=    25.0178
Eigenvalues:    24.9905    30.0839    35.4104
  29  H    Isotropic =    30.9756   Anisotropy =    10.2644
XX=    29.3113   YX=    -2.4244   ZX=    -3.3753
XY=    -2.8839   YY=    31.6034   ZY=     4.5692
XZ=    -3.2318   YZ=     3.2425   ZZ=    32.0120
Eigenvalues:    27.0922    28.0159    37.8185
  30  H    Isotropic =    30.5678   Anisotropy =     8.7416
XX=    30.2350   YX=    -2.8372   ZX=     2.3606
XY=    -3.7194   YY=    32.8339   ZY=    -2.6918
XZ=     2.5853   YZ=    -1.6901   ZZ=    28.6345
Eigenvalues:    26.8274    28.4805    36.3955
  31  H    Isotropic =    25.3649   Anisotropy =     6.9677
XX=    28.1200   YX=     2.3579   ZX=    -1.1602
XY=     2.4401   YY=    26.3850   ZY=    -0.7388
XZ=    -0.9135   YZ=    -0.8970   ZZ=    21.5897
Eigenvalues:    21.3816    24.7030    30.0100
  32  H    Isotropic =    25.4421   Anisotropy =     7.3616
XX=    30.0584   YX=    -0.4510   ZX=    -1.4845
XY=    -0.1294   YY=    24.7393   ZY=     0.1598
XZ=    -1.5943   YZ=     0.6067   ZZ=    21.5285
Eigenvalues:    21.2285    24.7479    30.3498
  33  H    Isotropic =    25.8220   Anisotropy =    20.4034
XX=    38.3300   YX=     2.2324   ZX=    -2.6027
XY=     4.0679   YY=    23.3589   ZY=    -1.6834
XZ=    -3.7435   YZ=    -0.1520   ZZ=    15.7770
Eigenvalues:    15.3090    22.7327    39.4242
  34  H    Isotropic =    30.2411   Anisotropy =    15.2212
XX=    37.0918   YX=     6.6411   ZX=    -0.6093
```

```
XY=     6.5591   YY=    25.4438   ZY=    -3.1307
XZ=    -0.9574   YZ=    -2.8560   ZZ=    28.1879
Eigenvalues:    21.5636    28.7712    40.3886
  35  H    Isotropic =    29.8765   Anisotropy =     7.9141
XX=    33.7554   YX=    -3.6277   ZX=    -0.8139
XY=    -1.1158   YY=    31.0086   ZY=    -0.6566
XZ=    -0.8863   YZ=    -0.0831   ZZ=    24.8655
Eigenvalues:    24.7234    29.7536    35.1526
  36  H    Isotropic =    29.4952   Anisotropy =     8.4210
XX=    31.9604   YX=     3.6862   ZX=     1.3050
XY=     1.9593   YY=    30.0573   ZY=     2.9690
XZ=     1.7281   YZ=     3.2446   ZZ=    26.4680
Eigenvalues:    24.6731    28.7033    35.1093
  37  H    Isotropic =    29.3698   Anisotropy =     8.5394
XX=    29.4217   YX=     1.2052   ZX=    -2.9153
XY=     0.6053   YY=    27.4504   ZY=    -2.6590
XZ=    -3.9030   YZ=    -3.5079   ZZ=    31.2373
Eigenvalues:    25.4146    27.6320    35.0627
  38  H    Isotropic =    29.9237   Anisotropy =     8.8630
XX=    26.3412   YX=    -0.4034   ZX=    -0.1816
XY=    -0.0014   YY=    35.2892   ZY=     0.5701
XZ=    -0.0335   YZ=     3.4964   ZZ=    28.1405
Eigenvalues:    26.3338    27.6049    35.8323
  39  H    Isotropic =    29.5565   Anisotropy =     4.7984
XX=    31.6906   YX=     1.1465   ZX=    -2.4728
XY=     0.7065   YY=    27.9327   ZY=     2.1929
XZ=    -1.4501   YZ=     2.4629   ZZ=    29.0462
Eigenvalues:    25.4720    30.4421    32.7554
  40  H    Isotropic =    29.8619   Anisotropy =     7.6026
XX=    28.6343   YX=    -0.3210   ZX=     3.7537
XY=    -0.4708   YY=    28.8981   ZY=     2.4443
XZ=     3.8951   YZ=     1.6851   ZZ=    32.0533
Eigenvalues:    25.4843    29.1711    34.9303
  41  H    Isotropic =    26.2782   Anisotropy =     5.4468
XX=    25.6519   YX=     1.6650   ZX=    -0.8015
XY=     0.9213   YY=    26.3512   ZY=    -1.3133
XZ=    -0.4430   YZ=    -4.4586   ZZ=    26.8315
Eigenvalues:    23.5404    25.3848    29.9094
  42  H    Isotropic =    26.4093   Anisotropy =     8.6002
XX=    25.2545   YX=     0.6860   ZX=    -0.6607
XY=     1.4516   YY=    27.1650   ZY=    -7.0566
XZ=    -1.2555   YZ=    -2.6516   ZZ=    26.8085
Eigenvalues:    22.1285    24.9567    32.1428
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 47.78 | 65.72 | 78.67 | 88.78 | 113.69 | 158.75 |
| intensities | 0.64 | 4.00 | 0.53 | 0.80 | 3.78 | 0.64 |
| reduc. mass | 1.26 | 1.06 | 1.11 | 1.51 | 1.53 | 0.48 |
| force const | 0.00 | 0.00 | 0.00 | 0.01 | 0.01 | 0.01 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 194.31 | 200.35 | 216.09 | 234.49 | 256.69 | 273.78 |
| intensities | 1.55 | 1.64 | 1.46 | 0.70 | 0.96 | 3.14 |
| reduc. mass | 0.71 | 0.24 | 0.87 | 1.01 | 0.78 | 1.12 |
| force const | 0.02 | 0.01 | 0.02 | 0.03 | 0.03 | 0.05 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 277.65 | 283.69 | 293.44 | 315.40 | 330.68 | 351.09 |
| intensities | 2.87 | 0.74 | 2.23 | 2.58 | 0.42 | 2.41 |
| reduc. mass | 0.33 | 0.75 | 0.22 | 0.50 | 0.91 | 1.23 |
| force const | 0.01 | 0.04 | 0.01 | 0.03 | 0.06 | 0.09 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 367.22 | 384.16 | 408.66 | 443.44 | 472.97 | 505.47 |
| intensities | 1.40 | 1.42 | 4.73 | 3.19 | 0.30 | 4.41 |
| reduc. mass | 1.04 | 1.17 | 0.69 | 1.57 | 0.73 | 0.55 |
| force const | 0.08 | 0.10 | 0.07 | 0.18 | 0.10 | 0.08 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 529.23 | 539.31 | 548.37 | 562.61 | 602.61 | 621.07 |
| intensities | 19.12 | 0.24 | 8.81 | 8.57 | 67.07 | 144.09 |
| reduc. mass | 1.68 | 0.82 | 0.82 | 0.59 | 0.47 | 0.58 |
| force const | 0.28 | 0.14 | 0.15 | 0.11 | 0.10 | 0.13 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 666.76 | 686.80 | 705.20 | 712.30 | 723.72 | 731.95 |
| intensities | 5.67 | 99.30 | 2.90 | 1.73 | 1.85 | 7.55 |
| reduc. mass | 0.87 | 0.60 | 1.47 | 0.29 | 1.11 | 1.29 |
| force const | 0.23 | 0.17 | 0.43 | 0.09 | 0.34 | 0.41 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 755.12 | 776.89 | 821.93 | 848.12 | 851.01 | 905.25 |
| intensities | 9.42 | 7.13 | 25.79 | 1.04 | 2.38 | 3.75 |
| reduc. mass | 1.64 | 0.50 | 0.84 | 0.82 | 2.72 | 0.49 |
| force const | 0.55 | 0.18 | 0.34 | 0.35 | 1.16 | 0.24 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 928.58 | 937.21 | 945.81 | 978.04 | 991.96 | 1019.28 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 3.26 | 3.30 | 5.48 | 14.24 | 7.82 | 3.52 |
| reduc. mass | 0.57 | 0.43 | 0.61 | 0.39 | 0.30 | 0.30 |
| force const | 0.29 | 0.22 | 0.32 | 0.22 | 0.17 | 0.18 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1029.45 | 1035.74 | 1047.16 | 1054.47 | 1074.17 | 1088.48 |
| intensities | 25.66 | 5.92 | 5.90 | 3.60 | 85.03 | 26.92 |
| reduc. mass | 0.54 | 0.64 | 0.34 | 0.22 | 0.40 | 0.95 |
| force const | 0.34 | 0.40 | 0.22 | 0.15 | 0.27 | 0.66 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1099.17 | 1125.46 | 1131.08 | 1161.06 | 1186.33 | 1212.55 |
| intensities | 4.70 | 14.16 | 79.74 | 17.02 | 9.22 | 89.03 |
| reduc. mass | 0.60 | 0.71 | 0.56 | 0.44 | 0.86 | 1.37 |
| force const | 0.42 | 0.53 | 0.42 | 0.35 | 0.72 | 1.18 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1221.39 | 1250.85 | 1252.85 | 1273.27 | 1292.88 | 1311.65 |
| intensities | 15.24 | 15.39 | 170.83 | 3.14 | 64.20 | 14.12 |
| reduc. mass | 0.73 | 0.35 | 1.14 | 0.32 | 0.98 | 0.76 |
| force const | 0.64 | 0.33 | 1.05 | 0.31 | 0.97 | 0.77 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1373.79 | 1401.02 | 1409.64 | 1436.55 | 1450.41 | 1469.80 |
| intensities | 47.41 | 152.69 | 353.07 | 22.19 | 57.97 | 118.72 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.43 | 0.65 | 0.92 | 0.38 | 3.34 | 0.73 |
| force const | 0.48 | 0.75 | 1.08 | 0.47 | 4.14 | 0.93 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1501.56 | 1506.13 | 1509.16 | 1520.20 | 1526.45 | 1540.32 |
| intensities | 7.98 | 32.05 | 20.13 | 37.70 | 212.12 | 51.33 |
| reduc. mass | 0.60 | 0.48 | 2.29 | 2.15 | 0.95 | 0.99 |
| force const | 0.80 | 0.65 | 3.07 | 2.93 | 1.31 | 1.39 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1563.04 | 1583.92 | 1592.60 | 1626.61 | 1631.61 | 1639.60 |
| intensities | 4.59 | 17.96 | 27.97 | 102.32 | 56.81 | 33.79 |
| reduc. mass | 0.59 | 0.80 | 0.52 | 0.33 | 0.35 | 0.21 |
| force const | 0.85 | 1.18 | 0.78 | 0.52 | 0.55 | 0.33 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1642.50 | 1654.69 | 1660.87 | 1662.93 | 1665.93 | 1666.86 |
| intensities | 20.54 | 28.72 | 29.80 | 26.10 | 12.16 | 8.47 |
| reduc. mass | 0.49 | 0.58 | 0.34 | 0.19 | 0.14 | 0.17 |
| force const | 0.78 | 0.93 | 0.56 | 0.32 | 0.23 | 0.28 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1669.57 | 1670.47 | 1671.88 | 1693.26 | 1695.93 | 1804.97 |
| intensities | 12.27 | 28.36 | 6.59 | 177.83 | 59.18 | 1049.82 |
| reduc. mass | 0.26 | 0.19 | 0.17 | 1.27 | 0.84 | 1.49 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 0.42 | 0.30 | 0.29 | 2.14 | 1.42 | 2.87 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1835.05 | 1887.99 | 3021.16 | 3024.10 | 3058.54 | 3065.60 |
| intensities | 457.45 | 19.71 | 291.66 | 405.38 | 141.80 | 743.89 |
| reduc. mass | 1.35 | 0.85 | 0.33 | 0.33 | 0.43 | 0.47 |
| force const | 2.69 | 1.78 | 1.78 | 1.75 | 2.39 | 2.58 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3073.13 | 3083.03 | 3091.45 | 3096.15 | 3107.63 | 3124.38 |
| intensities | 1103.54 | 54.75 | 296.84 | 451.59 | 56.96 | 531.23 |
| reduc. mass | 0.19 | 0.57 | 0.31 | 0.30 | 0.82 | 0.42 |
| force const | 1.07 | 3.18 | 1.74 | 1.72 | 4.68 | 2.40 |

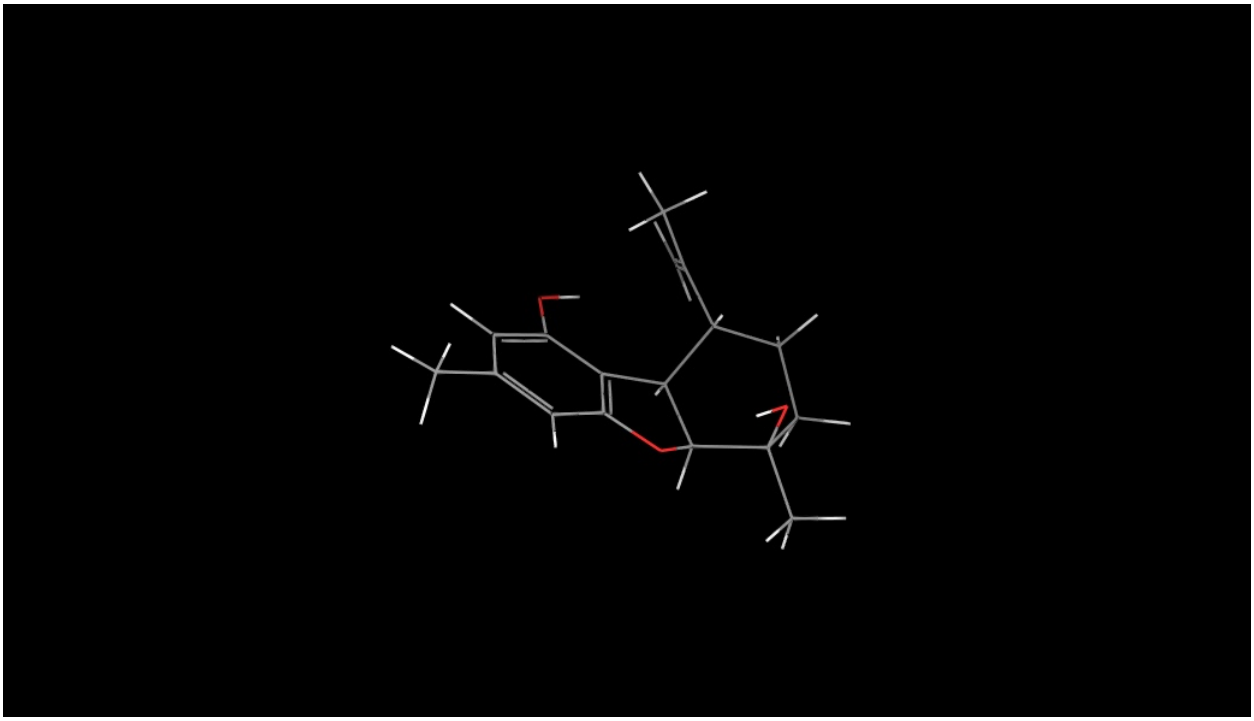
| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3127.71 | 3134.12 | 3140.39 | 3141.05 | 3144.94 | 3146.32 |
| intensities | 318.56 | 57.35 | 392.87 | 682.17 | 248.93 | 331.72 |
| reduc. mass | 0.54 | 0.40 | 0.54 | 0.38 | 0.33 | 0.57 |
| force const | 3.10 | 2.32 | 3.12 | 2.20 | 1.93 | 3.34 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3147.88 | 3154.81 | 3159.61 | 3196.54 | 3824.15 | 3831.35 |
| intensities | 299.76 | 327.42 | 298.02 | 341.54 | 369.73 | 18.36 |
| reduc. mass | 0.49 | 0.86 | 0.84 | 0.56 | 0.93 | 0.93 |
| force const | 2.89 | 5.05 | 4.91 | 3.36 | 8.03 | 8.06 |

Number of imaginary frequencies: 0

Conformation 3

Boltzmann Population = 18.9% (relative energy = 0.58 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.983134 hartrees

Total enthalpy, Htot (Utot + pV): -885.982189 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.044710 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.460700 | 2.255900 | 1.040900 |
| 2 | 6 | 0 | -3.511700 | 1.321300 | 2.264000 |
| 3 | 6 | 0 | -4.908700 | 1.229100 | 2.918500 |
| 4 | 6 | 0 | -5.660900 | 2.575000 | 2.793400 |

| | | | | | |
|---|---|---|---|---|---|
| 5 | 6 | 0 | -5.789500 | 3.028600 | 1.315000 |
| 6 | 6 | 0 | -4.808000 | 2.366800 | 0.333500 |
| 7 | 6 | 0 | -4.716200 | 3.183600 | -0.953700 |
| 8 | 6 | 0 | -4.859900 | 0.765000 | 4.365000 |
| 9 | 6 | 0 | -7.122600 | 2.517300 | 3.183200 |
| 10 | 6 | 0 | -7.892400 | 2.567500 | 2.021700 |
| 11 | 6 | 0 | -7.780600 | 2.416200 | 4.405400 |
| 12 | 6 | 0 | -9.181000 | 2.352200 | 4.422300 |
| 13 | 6 | 0 | -9.921300 | 2.384900 | 3.245300 |
| 14 | 6 | 0 | -9.270800 | 2.498900 | 2.007900 |
| 15 | 8 | 0 | -7.147000 | 2.378900 | 5.602000 |
| 16 | 8 | 0 | -7.128700 | 2.709100 | 0.893500 |
| 17 | 8 | 0 | -5.233900 | 1.048300 | 0.034300 |
| 18 | 6 | 0 | -11.425500 | 2.288500 | 3.285800 |
| 19 | 6 | 0 | -5.765200 | -0.384600 | 4.712500 |
| 20 | 6 | 0 | -4.091800 | 1.365200 | 5.282200 |
| 21 | 1 | 0 | -3.163000 | 3.267800 | 1.343600 |
| 22 | 1 | 0 | -2.708600 | 1.907700 | 0.326400 |
| 23 | 1 | 0 | -2.776700 | 1.659400 | 3.000200 |
| 24 | 1 | 0 | -3.215100 | 0.311600 | 1.968800 |
| 25 | 1 | 0 | -5.490400 | 0.499800 | 2.348000 |
| 26 | 1 | 0 | -5.108700 | 3.333400 | 3.363700 |
| 27 | 1 | 0 | -5.677100 | 4.119600 | 1.259600 |
| 28 | 1 | 0 | -4.083500 | 2.658800 | -1.673200 |
| 29 | 1 | 0 | -5.711700 | 3.311300 | -1.390300 |
| 30 | 1 | 0 | -4.293900 | 4.175800 | -0.767400 |
| 31 | 1 | 0 | -9.672400 | 2.275600 | 5.386500 |
| 32 | 1 | 0 | -9.822100 | 2.550100 | 1.075600 |
| 33 | 1 | 0 | -6.190400 | 2.296900 | 5.467000 |
| 34 | 1 | 0 | -6.185100 | 1.103800 | -0.135700 |
| 35 | 1 | 0 | -11.804700 | 2.415100 | 4.301500 |
| 36 | 1 | 0 | -11.884700 | 3.050900 | 2.650300 |
| 37 | 1 | 0 | -11.760400 | 1.313000 | 2.919600 |
| 38 | 1 | 0 | -5.742300 | -0.617800 | 5.779000 |
| 39 | 1 | 0 | -6.797300 | -0.157500 | 4.423000 |
| 40 | 1 | 0 | -5.465200 | -1.275200 | 4.149100 |
| 41 | 1 | 0 | -4.083900 | 1.031500 | 6.315700 |
| 42 | 1 | 0 | -3.433000 | 2.192000 | 5.030100 |

---

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 154.1725 Anisotropy = 27.6606

XX= 152.2476 YX= 5.8198 ZX= -9.0861

XY= 2.9602 YY= 171.1695 ZY= -3.6269

XZ= -4.7948 YZ= -1.2507 ZZ= 139.1005

Eigenvalues: 136.1071 153.7976 172.6130

2 C Isotropic = 157.7120 Anisotropy = 25.0096

XX= 173.3900 YX= -2.9543 ZX= -3.1331

XY= -2.6914 YY= 165.5023 ZY= -0.5512

```
XZ=    -2.9920   YZ=    -6.4587   ZZ=   134.2437
Eigenvalues:   133.5715   165.1794   174.3851
   3  C    Isotropic =   142.6605   Anisotropy =    14.5324
XX=   147.4539   YX=    -7.6557   ZX=     3.9006
XY=     0.4232   YY=   148.7291   ZY=     1.2085
XZ=     8.3165   YZ=     0.8161   ZZ=   131.7984
Eigenvalues:   129.4548   146.1778   152.3487
   4  C    Isotropic =   133.5223   Anisotropy =    27.1284
XX=   132.1411   YX=     6.2404   ZX=     2.3376
XY=    -5.4240   YY=   149.4688   ZY=    -0.2730
XZ=     6.5794   YZ=    16.5039   ZZ=   118.9569
Eigenvalues:   115.8328   133.1261   151.6078
   5  C    Isotropic =    96.7720   Anisotropy =    57.9141
XX=   118.7601   YX=    14.6264   ZX=   -13.3361
XY=    12.5933   YY=   101.2086   ZY=   -20.2967
XZ=   -22.1656   YZ=   -15.7831   ZZ=    70.3474
Eigenvalues:    59.9046    95.0301   135.3814
   6  C    Isotropic =   116.4127   Anisotropy =    47.9678
XX=    96.8968   YX=    -5.2830   ZX=   -11.8553
XY=    -2.4355   YY=   105.6215   ZY=    -1.4160
XZ=    -6.4629   YZ=     2.7255   ZZ=   146.7198
Eigenvalues:    94.0861   106.7608   148.3912
   7  C    Isotropic =   157.6746   Anisotropy =    46.4857
XX=   145.0811   YX=   -20.2426   ZX=    -4.3571
XY=   -22.2494   YY=   172.9235   ZY=    13.9231
XZ=     0.2492   YZ=    10.9558   ZZ=   155.0193
Eigenvalues:   132.7383   151.6204   188.6651
   8  C    Isotropic =    13.8137   Anisotropy =   216.7860
XX=    55.5831   YX=    80.8758   ZX=   100.6059
XY=    82.5178   YY=   -16.0730   ZY=   -12.6299
XZ=   105.7917   YZ=     0.5184   ZZ=     1.9310
Eigenvalues:  -113.9928    -2.9039   158.3377
   9  C    Isotropic =    72.6367   Anisotropy =   100.8398
XX=    26.4810   YX=     2.9680   ZX=    12.8743
XY=   -19.1105   YY=    64.9952   ZY=    27.2377
XZ=    19.9918   YZ=    32.3999   ZZ=   126.4339
Eigenvalues:    19.6267    58.4202   139.8632
  10  C    Isotropic =    20.3776   Anisotropy =   104.6143
XX=   -25.7198   YX=    38.9479   ZX=     6.6319
XY=    52.3914   YY=     1.2726   ZY=    17.8651
XZ=     0.3370   YZ=    14.8404   ZZ=    85.5802
Eigenvalues:   -60.1873    31.1996    90.1205
  11  C    Isotropic =    26.4718   Anisotropy =   137.8086
XX=    12.6518   YX=    -8.9369   ZX=    14.8176
XY=    -0.3570   YY=   -34.8247   ZY=    49.1798
XZ=    16.4653   YZ=    46.1950   ZZ=   101.5884
Eigenvalues:   -51.1710    12.2423   118.3442
  12  C    Isotropic =    73.9620   Anisotropy =   113.1677
XX=    26.2077   YX=    35.7812   ZX=     3.8654
XY=    45.3762   YY=    54.9430   ZY=    24.8524
XZ=     9.0625   YZ=    22.8809   ZZ=   140.7351
Eigenvalues:    -2.9968    75.4756   149.4071
```

```
  13  C    Isotropic =    40.6728   Anisotropy =   194.2800
XX=   -42.6797   YX=   -12.0101   ZX=    30.9845
XY=   -18.6943   YY=    14.5410   ZY=    52.3430
XZ=    28.9888   YZ=    50.8473   ZZ=   150.1573
Eigenvalues:   -56.0880     7.9137   170.1929
  14  C    Isotropic =    82.3662   Anisotropy =   121.3217
XX=    77.8554   YX=     6.0723   ZX=    10.6754
XY=    -6.0347   YY=    20.3481   ZY=    44.0044
XZ=    17.7827   YZ=    38.7447   ZZ=   148.8951
Eigenvalues:     7.9500    75.9012   163.2474
  15  O    Isotropic =   197.1835   Anisotropy =    82.5281
XX=   141.8867   YX=    14.7559   ZX=     5.9712
XY=    10.9897   YY=   202.8006   ZY=     9.3789
XZ=    33.4748   YZ=   -32.6188   ZZ=   246.8631
Eigenvalues:   135.0604   204.2879   252.2022
  16  O    Isotropic =   194.5531   Anisotropy =   110.7845
XX=   221.2796   YX=   -71.4995   ZX=    23.2398
XY=   -42.8007   YY=   179.5123   ZY=    18.4670
XZ=    26.1362   YZ=   -34.0355   ZZ=   182.8673
Eigenvalues:   138.0367   177.2132   268.4095
  17  O    Isotropic =   267.2998   Anisotropy =    29.1214
XX=   273.0013   YX=     3.8594   ZX=   -21.0336
XY=     3.0167   YY=   267.5295   ZY=    17.7127
XZ=   -16.2474   YZ=    -9.0547   ZZ=   261.3686
Eigenvalues:   246.2255   268.9598   286.7141
  18  C    Isotropic =   163.9429   Anisotropy =    41.3583
XX=   186.8799   YX=     7.8632   ZX=    -4.8079
XY=    10.7634   YY=   158.9244   ZY=    -4.8449
XZ=   -10.8104   YZ=    -6.1404   ZZ=   146.0244
Eigenvalues:   143.5310   156.7827   191.5151
  19  C    Isotropic =   157.1110   Anisotropy =    42.7428
XX=   156.5339   YX=   -13.0346   ZX=   -18.3494
XY=    -9.9916   YY=   154.1661   ZY=     9.8659
XZ=   -19.5068   YZ=    12.0223   ZZ=   160.6331
Eigenvalues:   139.3532   146.3736   185.6062
  20  C    Isotropic =    72.7562   Anisotropy =   131.0925
XX=    90.9010   YX=    65.3244   ZX=    60.2199
XY=    71.2462   YY=    38.9352   ZY=   -24.4865
XZ=    60.8554   YZ=   -31.2513   ZZ=    88.4325
Eigenvalues:   -36.0210    94.1385   160.1512
  21  H    Isotropic =    30.3672   Anisotropy =     8.0415
XX=    28.7084   YX=    -0.2526   ZX=    -4.3390
XY=    -0.0063   YY=    29.7057   ZY=    -0.5504
XZ=    -4.7159   YZ=    -1.3216   ZZ=    32.6874
Eigenvalues:    25.6564    29.7170    35.7282
  22  H    Isotropic =    29.8871   Anisotropy =     8.8432
XX=    35.3817   YX=    -1.5746   ZX=     1.1184
XY=    -1.2712   YY=    29.4155   ZY=     0.4425
XZ=     1.0043   YZ=     0.5612   ZZ=    24.8639
Eigenvalues:    24.6681    29.2105    35.7825
  23  H    Isotropic =    30.2895   Anisotropy =     8.5164
XX=    30.2066   YX=     0.9518   ZX=    -2.7137
```

```
XY=     0.9213   YY=    34.6592   ZY=    -3.0006
XZ=    -1.5544   YZ=    -2.8175   ZZ=    26.0028
Eigenvalues:    24.5428    30.3587    35.9671
  24  H    Isotropic =    29.7492   Anisotropy =     9.0256
XX=    31.2132   YX=     0.4423   ZX=     4.0339
XY=     1.1228   YY=    28.2493   ZY=     3.6270
XZ=     4.3266   YZ=     2.8915   ZZ=    29.7852
Eigenvalues:    24.8035    28.6779    35.7663
  25  H    Isotropic =    28.7614   Anisotropy =     4.8193
XX=    27.5891   YX=    -3.4710   ZX=    -1.3561
XY=    -2.3473   YY=    29.7616   ZY=    -0.4322
XZ=    -0.3456   YZ=     1.1064   ZZ=    28.9335
Eigenvalues:    25.4933    28.8166    31.9742
  26  H    Isotropic =    28.6601   Anisotropy =     4.3274
XX=    27.5029   YX=     0.3708   ZX=     0.7485
XY=    -1.4231   YY=    28.3705   ZY=    -1.7014
XZ=    -0.5590   YZ=    -2.4978   ZZ=    30.1068
Eigenvalues:    26.7595    27.6757    31.5451
  27  H    Isotropic =    27.3982   Anisotropy =     4.8249
XX=    25.9009   YX=    -0.1592   ZX=    -1.4208
XY=    -1.2792   YY=    27.5440   ZY=     0.9366
XZ=    -2.2381   YZ=     2.2039   ZZ=    28.7497
Eigenvalues:    25.0058    26.5741    30.6148
  28  H    Isotropic =    30.5931   Anisotropy =     9.2333
XX=    33.2577   YX=    -3.3522   ZX=     2.1627
XY=    -4.6680   YY=    30.8810   ZY=    -1.3244
XZ=     1.9706   YZ=    -0.2341   ZZ=    27.6405
Eigenvalues:    26.8142    28.2165    36.7486
  29  H    Isotropic =    30.0966   Anisotropy =     8.2867
XX=    29.5069   YX=    -0.3320   ZX=    -0.5755
XY=     0.9775   YY=    35.5739   ZY=     0.0466
XZ=    -0.4764   YZ=     1.1272   ZZ=    25.2090
Eigenvalues:    25.1087    29.5601    35.6211
  30  H    Isotropic =    30.8967   Anisotropy =     9.9082
XX=    28.6722   YX=    -2.0410   ZX=    -3.2047
XY=    -2.2620   YY=    30.3062   ZY=     3.8808
XZ=    -3.3679   YZ=     2.7952   ZZ=    33.7117
Eigenvalues:    26.9178    28.2702    37.5022
  31  H    Isotropic =    25.3128   Anisotropy =     6.8043
XX=    27.3472   YX=     2.3768   ZX=    -0.8955
XY=     2.5260   YY=    26.3886   ZY=    -1.8573
XZ=    -0.5577   YZ=    -2.3290   ZZ=    22.2026
Eigenvalues:    21.3211    24.7683    29.8490
  32  H    Isotropic =    25.3739   Anisotropy =     7.3553
XX=    30.1253   YX=     0.2003   ZX=    -0.9467
XY=     0.6590   YY=    24.6116   ZY=    -0.9270
XZ=    -0.9951   YZ=    -0.5238   ZZ=    21.3848
Eigenvalues:    21.1461    24.6982    30.2775
  33  H    Isotropic =    25.8573   Anisotropy =    19.0741
XX=    36.2243   YX=     4.3341   ZX=     3.1681
XY=     6.3461   YY=    25.2543   ZY=    -2.0794
XZ=     1.9104   YZ=     0.1851   ZZ=    16.0934
```

```
Eigenvalues:    15.4776    23.5209    38.5734
  34  H    Isotropic =    29.9865   Anisotropy =    15.4297
XX=    33.9979   YX=     7.3937   ZX=    -1.2842
XY=     7.3651   YY=    26.7841   ZY=    -5.2835
XZ=    -2.1535   YZ=    -4.9723   ZZ=    29.1774
Eigenvalues:    20.6186    29.0679    40.2730
  35  H    Isotropic =    29.8433   Anisotropy =     7.9189
XX=    34.5408   YX=    -2.7091   ZX=     1.1332
XY=    -0.2554   YY=    29.5298   ZY=    -2.0753
XZ=     0.4615   YZ=    -1.7530   ZZ=    25.4593
Eigenvalues:    24.6966    29.7107    35.1226
  36  H    Isotropic =    29.4757   Anisotropy =     8.4055
XX=    30.6237   YX=     3.6062   ZX=     0.2051
XY=     2.0724   YY=    32.6351   ZY=     1.8319
XZ=     1.0639   YZ=     2.3536   ZZ=    25.1683
Eigenvalues:    24.6197    28.7281    35.0794
  37  H    Isotropic =    29.3396   Anisotropy =     8.5548
XX=    29.5743   YX=     1.2540   ZX=    -3.0423
XY=     0.4056   YY=    26.3529   ZY=    -1.8510
XZ=    -3.6053   YZ=    -2.7878   ZZ=    32.0915
Eigenvalues:    25.4905    27.4854    35.0428
  38  H    Isotropic =    29.9323   Anisotropy =     8.5127
XX=    28.5070   YX=    -3.8541   ZX=    -0.7862
XY=    -2.4009   YY=    33.3500   ZY=     0.6008
XZ=    -1.5658   YZ=     3.4916   ZZ=    27.9400
Eigenvalues:    26.9030    27.2865    35.6074
  39  H    Isotropic =    30.0183   Anisotropy =     5.5414
XX=    31.4595   YX=     2.8409   ZX=    -1.6541
XY=     2.1429   YY=    30.1155   ZY=     2.1188
XZ=    -0.0886   YZ=     3.8669   ZZ=    28.4799
Eigenvalues:    25.3575    30.9849    33.7126
  40  H    Isotropic =    30.0000   Anisotropy =     8.0622
XX=    27.7093   YX=    -0.6395   ZX=     1.4442
XY=    -0.7557   YY=    27.9598   ZY=     2.5687
XZ=     1.9675   YZ=     2.1613   ZZ=    34.3309
Eigenvalues:    26.1263    28.4988    35.3748
  41  H    Isotropic =    26.3089   Anisotropy =     5.5550
XX=    25.0944   YX=     2.3183   ZX=    -0.5562
XY=     1.0603   YY=    27.9908   ZY=    -1.2219
XZ=     0.6868   YZ=    -3.7257   ZZ=    25.8416
Eigenvalues:    23.4811    25.4335    30.0123
  42  H    Isotropic =    26.3621   Anisotropy =     8.4296
XX=    25.2424   YX=     0.3389   ZX=     0.8305
XY=     2.5440   YY=    29.1166   ZY=    -6.4641
XZ=    -0.2171   YZ=    -2.2727   ZZ=    24.7272
Eigenvalues:    21.7287    25.3757    31.9819
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 52.62 | 74.49 | 82.55 | 95.16 | 115.88 | 153.11 |
| intensities | 0.49 | 1.31 | 1.06 | 0.02 | 2.60 | 2.00 |
| reduc. mass | 1.18 | 0.78 | 0.26 | 0.86 | 1.89 | 1.27 |
| force const | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.02 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 171.21 | 205.36 | 215.46 | 225.38 | 247.97 | 261.93 |
| intensities | 0.88 | 1.52 | 1.83 | 0.85 | 0.69 | 1.47 |
| reduc. mass | 0.67 | 0.75 | 0.47 | 1.34 | 0.78 | 0.81 |
| force const | 0.01 | 0.02 | 0.01 | 0.04 | 0.03 | 0.03 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 271.97 | 283.03 | 289.71 | 295.04 | 332.32 | 336.14 |
| intensities | 7.95 | 0.77 | 0.76 | 0.47 | 0.29 | 5.07 |
| reduc. mass | 1.91 | 0.64 | 0.45 | 0.33 | 0.90 | 1.45 |
| force const | 0.08 | 0.03 | 0.02 | 0.02 | 0.06 | 0.10 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 359.36 | 408.93 | 421.51 | 445.07 | 481.57 | 490.19 |
| intensities | 2.41 | 0.48 | 1.40 | 3.21 | 11.44 | 0.08 |
| reduc. mass | 0.98 | 1.07 | 0.55 | 0.87 | 0.72 | 0.92 |
| force const | 0.07 | 0.10 | 0.06 | 0.10 | 0.10 | 0.13 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 523.42 | 528.65 | 551.38 | 566.35 | 608.38 | 621.73 |
| intensities | 14.25 | 10.40 | 1.64 | 12.48 | 111.92 | 38.18 |
| reduc. mass | 0.99 | 2.38 | 0.78 | 0.91 | 0.61 | 0.70 |
| force const | 0.16 | 0.39 | 0.14 | 0.17 | 0.13 | 0.16 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 661.22 | 670.00 | 699.09 | 706.47 | 713.64 | 746.98 |
| intensities | 86.85 | 15.02 | 55.64 | 10.98 | 0.76 | 7.56 |
| reduc. mass | 0.36 | 0.87 | 0.70 | 0.89 | 0.33 | 1.10 |
| force const | 0.09 | 0.23 | 0.20 | 0.26 | 0.10 | 0.36 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 759.66 | 778.69 | 822.93 | 829.05 | 844.99 | 909.11 |
| intensities | 1.64 | 0.73 | 5.52 | 3.08 | 6.97 | 2.64 |
| reduc. mass | 0.81 | 0.47 | 1.26 | 2.69 | 0.80 | 0.57 |
| force const | 0.28 | 0.17 | 0.50 | 1.09 | 0.34 | 0.28 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 937.20 | 949.77 | 964.74 | 991.67 | 1006.81 | 1028.12 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 4.23 | 2.07 | 12.28 | 9.79 | 4.99 | 33.25 |
| reduc. mass | 0.33 | 0.58 | 1.09 | 0.46 | 0.31 | 0.49 |
| force const | 0.17 | 0.31 | 0.60 | 0.27 | 0.19 | 0.30 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1038.29 | 1052.01 | 1058.27 | 1061.63 | 1071.47 | 1093.65 |
| intensities | 4.26 | 2.71 | 18.64 | 10.62 | 73.36 | 10.28 |
| reduc. mass | 0.24 | 0.27 | 0.43 | 0.30 | 0.50 | 0.42 |
| force const | 0.15 | 0.17 | 0.29 | 0.20 | 0.34 | 0.29 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1099.35 | 1122.50 | 1148.45 | 1168.80 | 1178.78 | 1199.99 |
| intensities | 14.34 | 8.88 | 114.99 | 7.45 | 15.18 | 63.25 |
| reduc. mass | 0.42 | 0.62 | 0.84 | 0.41 | 0.97 | 1.22 |
| force const | 0.30 | 0.46 | 0.66 | 0.33 | 0.79 | 1.04 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1228.37 | 1253.30 | 1257.51 | 1283.27 | 1301.73 | 1306.00 |
| intensities | 30.44 | 43.12 | 87.70 | 0.08 | 84.65 | 23.59 |
| reduc. mass | 0.66 | 0.30 | 1.08 | 0.36 | 1.04 | 0.72 |
| force const | 0.58 | 0.28 | 1.01 | 0.35 | 1.04 | 0.72 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1374.76 | 1388.46 | 1407.93 | 1434.21 | 1456.15 | 1470.85 |
| intensities | 12.36 | 108.12 | 327.92 | 86.77 | 59.68 | 104.18 |

reduc. mass 0.45 0.63 0.80 1.34 0.53 1.20

force const 0.50 0.72 0.93 1.62 0.67 1.53

vibration # 73 74 75 76 77 78

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frequencies 1505.16 1507.30 1515.95 1523.26 1524.74 1534.55

intensities 39.39 3.73 8.45 45.37 189.23 7.66

reduc. mass 0.65 0.67 0.99 1.46 0.95 0.61

force const 0.87 0.89 1.35 2.00 1.30 0.85

C1 X 0.03454 0.00622 -0.01479 -0.04146 -0.03995 -0.06018

vibration # 79 80 81 82 83 84

-------- -------- -------- -------- -------- --------

frequencies 1561.55 1566.64 1590.35 1630.65 1634.23 1641.59

intensities 39.07 22.94 52.32 8.19 29.39 35.66

reduc. mass 0.46 0.44 0.78 0.74 0.30 0.18

force const 0.66 0.64 1.16 1.16 0.47 0.29

vibration # 85 86 87 88 89 90

-------- -------- -------- -------- -------- --------

frequencies 1645.51 1659.94 1661.64 1664.84 1665.54 1667.97

intensities 102.63 26.71 84.05 9.90 7.21 10.57

reduc. mass 0.49 0.31 0.26 0.22 0.21 0.14

force const 0.78 0.51 0.42 0.36 0.35 0.23

vibration # 91 92 93 94 95 96

-------- -------- -------- -------- -------- --------

frequencies 1668.05 1672.40 1680.08 1686.29 1708.69 1803.69

intensities 7.63 1.54 31.27 78.78 66.43 928.22

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.18 | 0.21 | 0.55 | 0.57 | 1.36 | 1.55 |
| force const | 0.30 | 0.34 | 0.91 | 0.96 | 2.34 | 2.96 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1846.05 | 1892.80 | 3022.06 | 3025.10 | 3036.48 | 3061.14 |
| intensities | 383.23 | 26.49 | 466.98 | 300.82 | 1009.64 | 374.22 |
| reduc. mass | 1.40 | 0.90 | 0.26 | 0.21 | 0.23 | 0.36 |
| force const | 2.81 | 1.90 | 1.42 | 1.14 | 1.26 | 1.97 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3071.90 | 3082.51 | 3085.81 | 3109.07 | 3113.72 | 3125.39 |
| intensities | 269.71 | 432.80 | 150.40 | 37.51 | 494.07 | 135.42 |
| reduc. mass | 0.30 | 0.46 | 0.46 | 0.52 | 0.18 | 0.26 |
| force const | 1.68 | 2.57 | 2.56 | 2.93 | 1.00 | 1.47 |

| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3126.20 | 3136.60 | 3137.16 | 3140.32 | 3146.91 | 3148.76 |
| intensities | 873.39 | 460.87 | 401.66 | 62.95 | 409.00 | 24.42 |
| reduc. mass | 0.23 | 0.38 | 0.27 | 0.18 | 0.23 | 0.26 |
| force const | 1.35 | 2.19 | 1.56 | 1.03 | 1.31 | 1.53 |

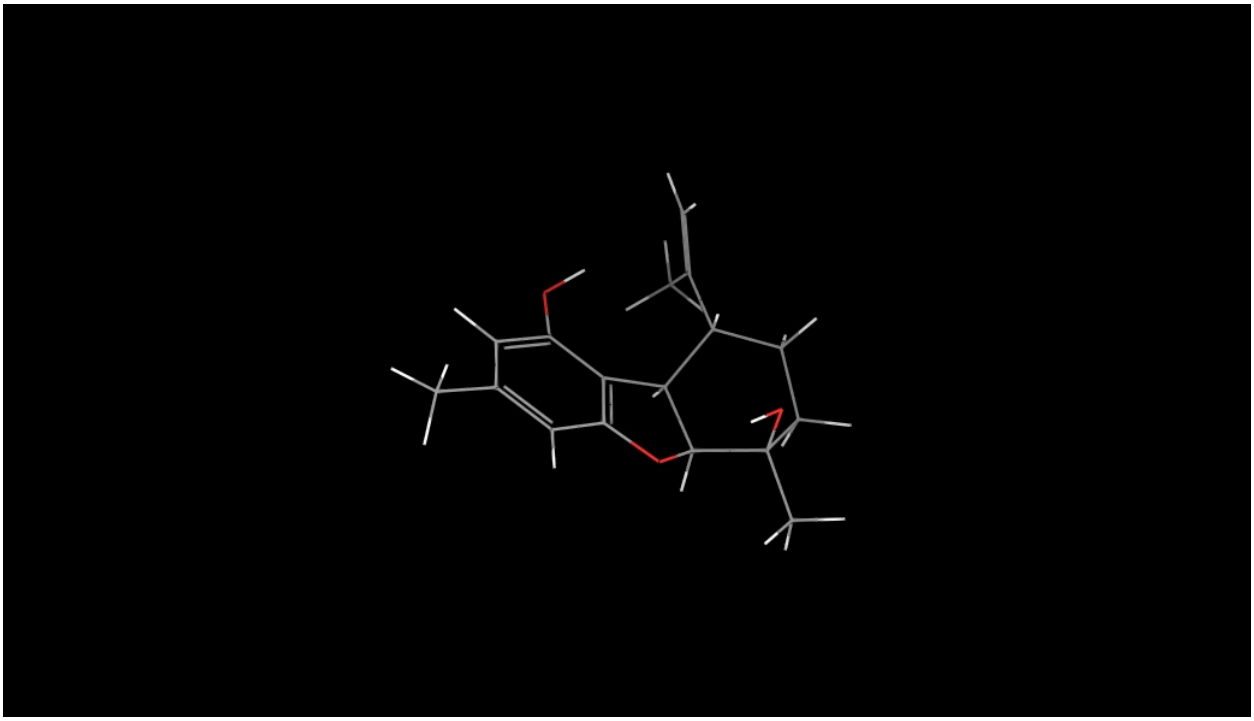
| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3151.65 | 3156.76 | 3193.08 | 3203.43 | 3822.95 | 3831.29 |
| intensities | 471.77 | 586.86 | 135.86 | 276.07 | 157.83 | 55.09 |
| reduc. mass | 0.21 | 0.39 | 0.39 | 0.22 | 0.70 | 0.70 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 1.22 | 2.31 | 2.35 | 1.31 | 6.05 | 6.08 |

Number of imaginary frequencies: 0

Conformation 4

Boltzmann Population = 18.9% (relative energy = 0.58 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.980277 hartrees

Total enthalpy, Htot (Utot + pV): -885.979333 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.041789 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -3.486500 | 2.159500 | 1.043400 |
| 2 | 6 | 0 | -3.566800 | 1.187800 | 2.228800 |
| 3 | 6 | 0 | -4.931200 | 1.190200 | 2.971900 |

| | | | | | |
|---|---|---|---|---|---|
| 4 | 6 | 0 | -5.690100 | 2.531000 | 2.831100 |
| 5 | 6 | 0 | -5.760600 | 3.047000 | 1.362000 |
| 6 | 6 | 0 | -4.840200 | 2.331900 | 0.365600 |
| 7 | 6 | 0 | -4.739900 | 3.129300 | -0.932600 |
| 8 | 6 | 0 | -4.716200 | 0.801300 | 4.421300 |
| 9 | 6 | 0 | -7.168600 | 2.459400 | 3.167500 |
| 10 | 6 | 0 | -7.903700 | 2.670900 | 2.003000 |
| 11 | 6 | 0 | -7.874400 | 2.255400 | 4.351000 |
| 12 | 6 | 0 | -9.272500 | 2.299500 | 4.334700 |
| 13 | 6 | 0 | -9.979400 | 2.518600 | 3.155200 |
| 14 | 6 | 0 | -9.284400 | 2.704500 | 1.954800 |
| 15 | 8 | 0 | -7.264900 | 2.054700 | 5.556400 |
| 16 | 8 | 0 | -7.114100 | 2.875200 | 0.905300 |
| 17 | 8 | 0 | -5.346000 | 1.034400 | 0.099400 |
| 18 | 6 | 0 | -11.487000 | 2.525600 | 3.155600 |
| 19 | 6 | 0 | -4.024600 | 1.794600 | 5.326000 |
| 20 | 6 | 0 | -5.125300 | -0.387100 | 4.879100 |
| 21 | 1 | 0 | -3.149700 | 3.150500 | 1.374400 |
| 22 | 1 | 0 | -2.754000 | 1.803900 | 0.312000 |
| 23 | 1 | 0 | -2.751300 | 1.410100 | 2.924100 |
| 24 | 1 | 0 | -3.400900 | 0.168000 | 1.874400 |
| 25 | 1 | 0 | -5.557200 | 0.428200 | 2.500900 |
| 26 | 1 | 0 | -5.185400 | 3.290300 | 3.439900 |
| 27 | 1 | 0 | -5.543000 | 4.122700 | 1.343300 |
| 28 | 1 | 0 | -4.154200 | 2.563700 | -1.661100 |
| 29 | 1 | 0 | -5.737700 | 3.306800 | -1.345500 |
| 30 | 1 | 0 | -4.259600 | 4.098500 | -0.767900 |
| 31 | 1 | 0 | -9.791800 | 2.147700 | 5.275300 |
| 32 | 1 | 0 | -9.800600 | 2.888500 | 1.019000 |
| 33 | 1 | 0 | -6.556300 | 1.405100 | 5.434600 |
| 34 | 1 | 0 | -6.288900 | 1.148200 | -0.086300 |
| 35 | 1 | 0 | -11.882400 | 2.693700 | 4.159100 |
| 36 | 1 | 0 | -11.877600 | 3.305400 | 2.496800 |
| 37 | 1 | 0 | -11.878400 | 1.568300 | 2.797500 |
| 38 | 1 | 0 | -3.139400 | 2.228500 | 4.851700 |
| 39 | 1 | 0 | -4.696300 | 2.624100 | 5.574300 |
| 40 | 1 | 0 | -3.716200 | 1.322900 | 6.261100 |
| 41 | 1 | 0 | -4.942800 | -0.696000 | 5.904700 |
| 42 | 1 | 0 | -5.644400 | -1.089900 | 4.234300 |

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SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 154.0129 Anisotropy = 24.5160

XX= 153.6165 YX= 7.6458 ZX= -8.5415

XY= 4.3312 YY= 168.1433 ZY= -0.4775

XZ= -2.0742 YZ= 1.4272 ZZ= 140.2791

Eigenvalues: 138.2161 153.4658 170.3569

2 C Isotropic = 161.0655 Anisotropy = 24.4491

XX= 174.4049 YX= -7.6684 ZX= 0.8994

XY= -4.4659 YY= 163.6892 ZY= 8.1661

XZ= -0.0312 YZ= 6.2509 ZZ= 145.1025

```
Eigenvalues:   142.4502   163.3814   177.3649
   3  C    Isotropic =   137.6528   Anisotropy =    14.2686
XX=   138.3095   YX=    -5.8256   ZX=     2.5872
XY=     4.2025   YY=   147.0628   ZY=     0.5512
XZ=     5.2990   YZ=    -1.2420   ZZ=   127.5861
Eigenvalues:   126.2920   139.5012   147.1652
   4  C    Isotropic =   141.3030   Anisotropy =    22.1178
XX=   154.4038   YX=     0.8734   ZX=    -0.6497
XY=    -6.8999   YY=   148.2513   ZY=     3.4408
XZ=     0.1542   YZ=    13.4371   ZZ=   121.2538
Eigenvalues:   118.8230   149.0377   156.0482
   5  C    Isotropic =    98.1647   Anisotropy =    59.9411
XX=   124.1154   YX=    15.8117   ZX=   -12.8131
XY=    14.1046   YY=   101.2068   ZY=   -14.3432
XZ=   -21.7672   YZ=   -11.9013   ZZ=    69.1718
Eigenvalues:    62.0945    94.2741   138.1254
   6  C    Isotropic =   116.6879   Anisotropy =    49.4367
XX=    96.8049   YX=    -4.1785   ZX=   -13.4275
XY=    -1.4785   YY=   105.9467   ZY=     0.0181
XZ=    -7.8391   YZ=     4.6535   ZZ=   147.3121
Eigenvalues:    94.1975   106.2204   149.6457
   7  C    Isotropic =   158.3272   Anisotropy =    45.8746
XX=   141.6829   YX=   -15.9774   ZX=    -3.6543
XY=   -17.8023   YY=   178.1349   ZY=    13.7355
XZ=     0.7157   YZ=    10.4782   ZZ=   155.1637
Eigenvalues:   134.5385   151.5327   188.9103
   8  C    Isotropic =    24.9355   Anisotropy =   197.4257
XX=   143.4377   YX=    18.3394   ZX=    39.6725
XY=    16.1568   YY=   -53.1714   ZY=    62.7021
XZ=    35.1741   YZ=    59.7692   ZZ=   -15.4599
Eigenvalues:   -98.6928    16.9466   156.5526
   9  C    Isotropic =    66.9761   Anisotropy =   107.5572
XX=    20.0264   YX=     6.1237   ZX=    21.2933
XY=   -17.7214   YY=    51.6306   ZY=    19.7909
XZ=    24.0644   YZ=    24.3946   ZZ=   129.2711
Eigenvalues:    12.6825    49.5648   138.6809
  10  C    Isotropic =    20.7075   Anisotropy =   104.0645
XX=   -15.7002   YX=    40.1309   ZX=    12.1864
XY=    53.2829   YY=    -9.1882   ZY=     4.7483
XZ=    13.3759   YZ=     5.8955   ZZ=    87.0108
Eigenvalues:   -59.4901    31.5287    90.0838
  11  C    Isotropic =    26.7610   Anisotropy =   131.4182
XX=    18.2765   YX=   -18.7323   ZX=    14.1850
XY=    -8.6873   YY=   -47.0372   ZY=    22.9494
XZ=    12.0565   YZ=    28.2976   ZZ=   109.0437
Eigenvalues:   -54.5159    20.4258   114.3732
  12  C    Isotropic =    69.1229   Anisotropy =   117.5304
XX=    31.5022   YX=    37.5389   ZX=     9.5110
XY=    50.3821   YY=    33.2511   ZY=    10.9143
XZ=    23.5495   YZ=     7.8200   ZZ=   142.6154
Eigenvalues:   -11.7753    71.6676   147.4765
  13  C    Isotropic =    41.1465   Anisotropy =   194.1429
```

```
XX=   -44.5677   YX=   -12.0887   ZX=    33.1587
XY=   -17.7583   YY=     6.3516   ZY=    30.2126
XZ=    31.4013   YZ=    25.8480   ZZ=   161.6557
Eigenvalues:   -55.6086     8.4731   170.5751
  14  C    Isotropic =    80.3375   Anisotropy =   122.8206
XX=    74.7770   YX=    -2.9697   ZX=    14.6528
XY=   -14.7739   YY=    10.4334   ZY=    25.0686
XZ=    20.9385   YZ=    19.6077   ZZ=   155.8021
Eigenvalues:     5.1585    73.6360   162.2179
  15  O    Isotropic =   215.9340   Anisotropy =    61.8567
XX=   167.7987   YX=     1.4117   ZX=    -1.3776
XY=     4.2032   YY=   226.8360   ZY=    13.8663
XZ=    38.1483   YZ=    -9.8321   ZZ=   253.1671
Eigenvalues:   163.9203   226.7098   257.1718
  16  O    Isotropic =   193.2748   Anisotropy =   110.4479
XX=   206.7795   YX=   -76.4093   ZX=    15.0818
XY=   -47.4174   YY=   195.1468   ZY=    14.3390
XZ=    15.1413   YZ=   -35.4601   ZZ=   177.8980
Eigenvalues:   138.6243   174.2933   266.9067
  17  O    Isotropic =   270.0788   Anisotropy =    30.3152
XX=   274.4001   YX=     2.4890   ZX=   -20.0248
XY=     3.0906   YY=   271.4108   ZY=    23.9343
XZ=   -18.8750   YZ=    -4.8116   ZZ=   264.4255
Eigenvalues:   245.9250   274.0225   290.2889
  18  C    Isotropic =   164.2794   Anisotropy =    40.7974
XX=   188.3006   YX=     6.9028   ZX=    -3.0547
XY=     9.0874   YY=   159.1560   ZY=    -2.1727
XZ=   -10.1289   YZ=    -4.4276   ZZ=   145.3815
Eigenvalues:   144.0730   157.2874   191.4776
  19  C    Isotropic =   167.7464   Anisotropy =    25.9483
XX=   159.1729   YX=     2.0937   ZX=    -4.0786
XY=     5.2134   YY=   168.0081   ZY=   -13.3738
XZ=    -5.2889   YZ=    -8.4957   ZZ=   176.0582
Eigenvalues:   157.7763   160.4176   185.0453
  20  C    Isotropic =    66.7459   Anisotropy =   112.4239
XX=   137.9044   YX=     7.1251   ZX=     6.5576
XY=     7.0724   YY=     2.1181   ZY=    60.1178
XZ=    15.1188   YZ=    58.9951   ZZ=    60.2152
Eigenvalues:   -35.0968    93.6393   141.6952
  21  H    Isotropic =    30.5409   Anisotropy =     7.8793
XX=    29.1505   YX=     0.0132   ZX=    -4.3215
XY=     0.3568   YY=    29.8873   ZY=    -0.0597
XZ=    -4.8457   YZ=    -0.7317   ZZ=    32.5848
Eigenvalues:    25.9716    29.8573    35.7938
  22  H    Isotropic =    29.9237   Anisotropy =     9.0162
XX=    34.9594   YX=    -2.4880   ZX=     1.2169
XY=    -2.1119   YY=    29.8998   ZY=     0.3824
XZ=     1.2123   YZ=     0.5304   ZZ=    24.9119
Eigenvalues:    24.6567    29.1798    35.9345
  23  H    Isotropic =    30.3606   Anisotropy =     7.9777
XX=    31.7221   YX=     1.4555   ZX=    -2.3814
XY=     1.7418   YY=    34.1086   ZY=    -2.3426
```

```
XZ=    -0.9269   YZ=    -2.3216   ZZ=    25.2510
Eigenvalues:    24.4578    30.9449    35.6791
  24  H    Isotropic =    29.9378   Anisotropy =     9.0107
XX=    30.2554   YX=    -0.3407   ZX=     4.6862
XY=     0.1865   YY=    28.0663   ZY=     2.8146
XZ=     4.5732   YZ=     1.9597   ZZ=    31.4918
Eigenvalues:    25.1782    28.6903    35.9449
  25  H    Isotropic =    28.4447   Anisotropy =     3.0104
XX=    27.1151   YX=    -1.5415   ZX=    -1.2430
XY=    -1.3558   YY=    29.4201   ZY=    -0.3967
XZ=     0.2005   YZ=     1.5348   ZZ=    28.7989
Eigenvalues:    26.3945    28.4879    30.4516
  26  H    Isotropic =    28.2007   Anisotropy =     5.6500
XX=    25.5327   YX=     0.7016   ZX=     0.9446
XY=    -0.7528   YY=    29.9154   ZY=    -1.7636
XZ=    -0.8744   YZ=    -3.0413   ZZ=    29.1542
Eigenvalues:    25.5323    27.1025    31.9674
  27  H    Isotropic =    27.3632   Anisotropy =     4.6638
XX=    25.4812   YX=    -0.0029   ZX=    -1.4521
XY=    -0.5928   YY=    27.5942   ZY=     1.0031
XZ=    -1.8353   YZ=     2.0397   ZZ=    29.0142
Eigenvalues:    24.8010    26.8163    30.4724
  28  H    Isotropic =    30.6188   Anisotropy =     9.2643
XX=    32.0928   YX=    -3.5915   ZX=     2.1446
XY=    -4.7758   YY=    31.9525   ZY=    -1.6941
XZ=     2.0526   YZ=    -0.5763   ZZ=    27.8111
Eigenvalues:    26.8206    28.2407    36.7950
  29  H    Isotropic =    30.0553   Anisotropy =     8.2588
XX=    29.8766   YX=     0.3545   ZX=    -0.4212
XY=     1.7570   YY=    35.3040   ZY=     0.3785
XZ=    -0.0360   YZ=     1.3136   ZZ=    24.9854
Eigenvalues:    24.8963    29.7085    35.5612
  30  H    Isotropic =    30.9007   Anisotropy =    10.0191
XX=    28.4150   YX=    -1.8888   ZX=    -3.0064
XY=    -2.1163   YY=    30.7242   ZY=     4.1462
XZ=    -3.2660   YZ=     3.1771   ZZ=    33.5627
Eigenvalues:    26.8964    28.2255    37.5800
  31  H    Isotropic =    25.1800   Anisotropy =     7.1413
XX=    27.6621   YX=     2.5368   ZX=    -0.9992
XY=     2.6408   YY=    26.1132   ZY=    -1.0978
XZ=    -0.9277   YZ=    -1.9624   ZZ=    21.7648
Eigenvalues:    21.2766    24.3226    29.9409
  32  H    Isotropic =    25.2741   Anisotropy =     7.5013
XX=    30.1586   YX=    -0.2441   ZX=    -1.0136
XY=     0.2062   YY=    24.5070   ZY=    -0.4007
XZ=    -1.0474   YZ=    -0.0529   ZZ=    21.1568
Eigenvalues:    21.0255    24.5219    30.2750
  33  H    Isotropic =    26.3719   Anisotropy =    22.8080
XX=    35.1582   YX=     3.7616   ZX=     8.0452
XY=     5.8386   YY=    24.7943   ZY=     3.2391
XZ=    10.2336   YZ=     5.3666   ZZ=    19.1631
Eigenvalues:    14.5848    22.9536    41.5772
```

```
  34  H    Isotropic =    30.0613   Anisotropy =    15.4918
XX=    35.2752   YX=     7.0459   ZX=    -1.5569
XY=     6.8647   YY=    26.0271   ZY=    -4.8978
XZ=    -2.2481   YZ=    -4.4798   ZZ=    28.8817
Eigenvalues:    20.8467    28.9481    40.3892
  35  H    Isotropic =    29.8093   Anisotropy =     8.0015
XX=    34.1873   YX=    -3.0266   ZX=     1.1685
XY=    -0.6161   YY=    29.9702   ZY=    -1.8609
XZ=     1.0384   YZ=    -1.5931   ZZ=    25.2703
Eigenvalues:    24.6776    29.6066    35.1436
  36  H    Isotropic =    29.5637   Anisotropy =     8.1789
XX=    31.1441   YX=     3.6563   ZX=     0.4934
XY=     1.7603   YY=    32.1574   ZY=     2.3125
XZ=     1.0752   YZ=     2.6345   ZZ=    25.3896
Eigenvalues:    24.5803    29.0945    35.0163
  37  H    Isotropic =    29.3524   Anisotropy =     8.7259
XX=    29.7307   YX=     1.1374   ZX=    -3.3317
XY=     0.5734   YY=    26.5575   ZY=    -1.6090
XZ=    -4.2381   YZ=    -2.2999   ZZ=    31.7690
Eigenvalues:    25.8163    27.0712    35.1697
  38  H    Isotropic =    29.8377   Anisotropy =     6.4469
XX=    31.6617   YX=    -1.0229   ZX=    -3.6027
XY=    -0.1036   YY=    29.9213   ZY=    -3.1062
XZ=    -3.8118   YZ=    -1.8412   ZZ=    27.9301
Eigenvalues:    24.5562    30.8213    34.1356
  39  H    Isotropic =    29.2296   Anisotropy =     5.3435
XX=    29.8395   YX=     0.9998   ZX=     3.3444
XY=     1.2102   YY=    28.3277   ZY=    -1.8916
XZ=     2.7961   YZ=    -1.5277   ZZ=    29.5217
Eigenvalues:    25.2833    29.6136    32.7920
  40  H    Isotropic =    29.9156   Anisotropy =     8.9442
XX=    26.5509   YX=     1.2727   ZX=    -0.9323
XY=     0.6394   YY=    35.7004   ZY=     0.0010
XZ=    -0.5865   YZ=    -1.4774   ZZ=    27.4955
Eigenvalues:    26.1033    27.7650    35.8784
  41  H    Isotropic =    26.5979   Anisotropy =     6.9035
XX=    25.4859   YX=    -0.7476   ZX=    -0.4723
XY=    -0.0064   YY=    26.8699   ZY=     2.1646
XZ=    -0.7962   YZ=     5.7255   ZZ=    27.4379
Eigenvalues:    23.1877    25.4058    31.2003
  42  H    Isotropic =    26.4619   Anisotropy =     7.2612
XX=    25.7137   YX=    -0.0528   ZX=    -1.1714
XY=    -1.1258   YY=    25.4787   ZY=     5.1473
XZ=     0.0767   YZ=     3.1294   ZZ=    28.1934
Eigenvalues:    22.4731    25.6099    31.3028
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 56.49 | 76.31 | 87.84 | 95.64 | 119.05 | 143.20 |
| intensities | 0.59 | 1.00 | 1.54 | 0.44 | 1.79 | 2.73 |
| reduc. mass | 1.60 | 0.83 | 0.26 | 1.02 | 2.39 | 1.65 |
| force const | 0.00 | 0.00 | 0.00 | 0.01 | 0.02 | 0.02 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 180.17 | 204.71 | 219.27 | 229.16 | 247.12 | 268.64 |
| intensities | 2.28 | 0.42 | 1.98 | 0.57 | 2.84 | 2.71 |
| reduc. mass | 0.67 | 1.08 | 1.32 | 1.22 | 0.76 | 0.46 |
| force const | 0.01 | 0.03 | 0.04 | 0.04 | 0.03 | 0.02 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 271.53 | 284.83 | 296.46 | 302.34 | 324.59 | 345.95 |
| intensities | 3.72 | 0.45 | 0.82 | 1.57 | 2.14 | 0.53 |
| reduc. mass | 0.63 | 0.41 | 0.23 | 0.46 | 1.75 | 0.84 |
| force const | 0.03 | 0.02 | 0.01 | 0.02 | 0.11 | 0.06 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

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| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 369.34 | 405.74 | 417.32 | 446.61 | 469.30 | 489.66 |
| intensities | 3.83 | 8.63 | 1.29 | 2.69 | 101.58 | 4.18 |
| reduc. mass | 0.72 | 1.22 | 0.70 | 0.90 | 0.56 | 0.73 |
| force const | 0.06 | 0.12 | 0.07 | 0.11 | 0.07 | 0.10 |

| | | | | | | |
|---|---|---|---|---|---|---|
| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |

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|---|---|---|---|---|---|---|
| frequencies | 509.53 | 525.40 | 535.08 | 553.56 | 576.01 | 613.29 |
| intensities | 11.70 | 3.59 | 0.57 | 15.50 | 14.72 | 34.57 |
| reduc. mass | 0.54 | 1.43 | 0.81 | 0.63 | 0.58 | 0.81 |
| force const | 0.08 | 0.23 | 0.14 | 0.11 | 0.11 | 0.18 |

| | | | | | | |
|---|---|---|---|---|---|---|
| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |

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|---|---|---|---|---|---|---|
| frequencies | 625.07 | 667.59 | 693.44 | 706.78 | 712.75 | 734.21 |
| intensities | 127.21 | 7.97 | 13.59 | 11.21 | 3.85 | 1.75 |
| reduc. mass | 0.72 | 0.95 | 0.82 | 1.51 | 0.42 | 1.84 |
| force const | 0.17 | 0.25 | 0.23 | 0.44 | 0.13 | 0.58 |

| | | | | | | |
|---|---|---|---|---|---|---|
| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |

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|---|---|---|---|---|---|---|
| frequencies | 756.88 | 776.17 | 790.50 | 818.44 | 835.79 | 911.63 |
| intensities | 3.58 | 6.10 | 6.63 | 12.84 | 15.27 | 9.39 |
| reduc. mass | 0.87 | 0.59 | 1.72 | 0.89 | 0.82 | 0.56 |
| force const | 0.29 | 0.21 | 0.63 | 0.35 | 0.34 | 0.27 |

| | | | | | | |
|---|---|---|---|---|---|---|
| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |

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|---|---|---|---|---|---|---|
| frequencies | 917.25 | 948.50 | 953.47 | 999.05 | 1006.27 | 1024.13 |
| intensities | 2.88 | 6.48 | 5.81 | 8.55 | 7.71 | 20.10 |
| reduc. mass | 0.49 | 0.52 | 1.49 | 0.49 | 0.20 | 0.21 |
| force const | 0.24 | 0.28 | 0.80 | 0.29 | 0.12 | 0.13 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1029.48 | 1029.53 | 1051.78 | 1062.23 | 1072.76 | 1093.02 |
| intensities | 12.30 | 9.57 | 7.20 | 1.70 | 7.82 | 103.41 |
| reduc. mass | 0.20 | 0.26 | 0.47 | 0.29 | 0.37 | 0.83 |
| force const | 0.12 | 0.16 | 0.30 | 0.19 | 0.25 | 0.59 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1094.68 | 1120.59 | 1139.11 | 1150.33 | 1172.97 | 1199.85 |
| intensities | 17.51 | 30.94 | 13.91 | 70.97 | 11.41 | 74.14 |
| reduc. mass | 0.57 | 0.34 | 0.58 | 0.57 | 0.31 | 1.19 |
| force const | 0.41 | 0.25 | 0.45 | 0.44 | 0.25 | 1.01 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1233.77 | 1246.78 | 1252.74 | 1281.64 | 1305.72 | 1318.71 |
| intensities | 29.46 | 67.12 | 89.10 | 1.99 | 101.70 | 8.14 |
| reduc. mass | 0.55 | 0.20 | 0.85 | 0.27 | 1.02 | 0.42 |
| force const | 0.49 | 0.19 | 0.78 | 0.26 | 1.03 | 0.43 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1380.56 | 1392.34 | 1400.47 | 1427.87 | 1444.31 | 1465.61 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 185.73 | 26.87 | 280.85 | 74.57 | 82.06 | 66.77 |
| reduc. mass | 0.67 | 0.46 | 0.60 | 0.78 | 2.10 | 1.04 |
| force const | 0.76 | 0.53 | 0.69 | 0.93 | 2.58 | 1.32 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1487.72 | 1498.49 | 1507.18 | 1521.68 | 1526.98 | 1541.30 |
| intensities | 23.56 | 50.67 | 33.30 | 17.37 | 250.86 | 20.38 |
| reduc. mass | 0.60 | 0.51 | 0.60 | 0.74 | 1.54 | 0.54 |
| force const | 0.79 | 0.68 | 0.80 | 1.01 | 2.11 | 0.75 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1562.19 | 1571.96 | 1605.86 | 1628.11 | 1634.65 | 1644.29 |
| intensities | 16.14 | 17.45 | 30.12 | 113.48 | 51.79 | 28.90 |
| reduc. mass | 0.56 | 0.65 | 0.86 | 0.24 | 0.24 | 0.26 |
| force const | 0.80 | 0.94 | 1.31 | 0.38 | 0.37 | 0.41 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1648.17 | 1650.52 | 1655.79 | 1660.20 | 1662.40 | 1665.10 |
| intensities | 145.69 | 136.61 | 3.38 | 8.32 | 18.79 | 10.50 |
| reduc. mass | 0.27 | 0.39 | 0.20 | 0.35 | 0.21 | 0.35 |
| force const | 0.43 | 0.62 | 0.33 | 0.57 | 0.34 | 0.57 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1666.31 | 1669.27 | 1675.60 | 1691.66 | 1702.06 | 1784.21 |
| intensities | 67.36 | 4.27 | 12.99 | 302.99 | 41.76 | 633.53 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.18 | 0.28 | 0.33 | 0.66 | 0.93 | 1.65 |
| force const | 0.30 | 0.46 | 0.55 | 1.11 | 1.59 | 3.10 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1835.03 | 1891.98 | 3022.80 | 3026.97 | 3047.36 | 3057.15 |
| intensities | 374.19 | 11.00 | 438.63 | 323.91 | 1057.39 | 195.64 |
| reduc. mass | 1.51 | 0.89 | 0.24 | 0.25 | 0.18 | 0.21 |
| force const | 2.99 | 1.87 | 1.28 | 1.36 | 1.00 | 1.16 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3071.38 | 3083.66 | 3091.54 | 3110.72 | 3117.84 | 3131.01 |
| intensities | 353.77 | 479.02 | 270.46 | 65.93 | 306.91 | 279.84 |
| reduc. mass | 0.42 | 0.80 | 0.72 | 0.70 | 0.26 | 0.28 |
| force const | 2.34 | 4.48 | 4.05 | 3.96 | 1.47 | 1.64 |

| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3134.49 | 3135.68 | 3140.24 | 3142.36 | 3146.46 | 3150.29 |
| intensities | 729.97 | 246.37 | 474.07 | 96.31 | 354.42 | 207.05 |
| reduc. mass | 0.12 | 0.39 | 0.43 | 0.33 | 0.19 | 0.20 |
| force const | 0.72 | 2.25 | 2.48 | 1.92 | 1.13 | 1.17 |

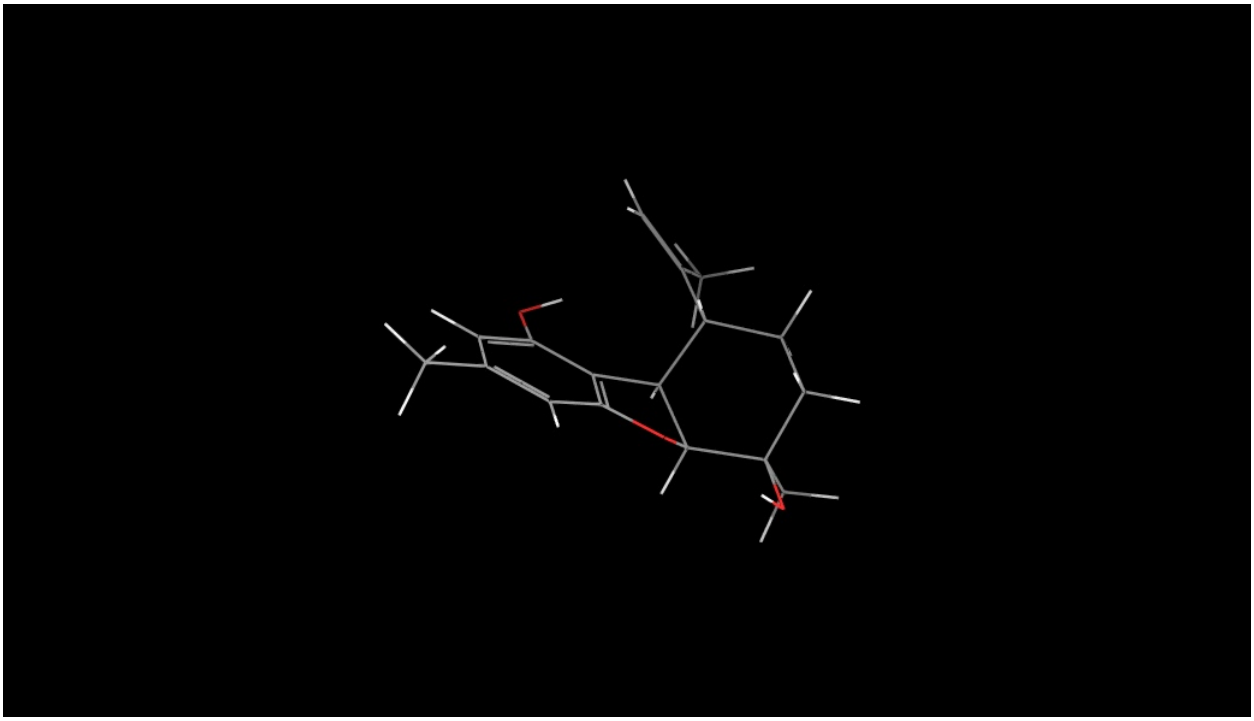
| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3155.05 | 3160.99 | 3190.32 | 3197.95 | 3828.74 | 3846.93 |
| intensities | 385.52 | 636.64 | 444.39 | 320.76 | 24.62 | 284.09 |
| reduc. mass | 0.27 | 0.52 | 0.17 | 0.54 | 0.95 | 0.95 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 1.58 | 3.05 | 1.02 | 3.23 | 8.18 | 8.25 |

Number of imaginary frequencies: 0

Conformation 5

Boltzmann Population = 1.0% (relative energy = 2.29 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.981795 hartrees

Total enthalpy, Htot (Utot + pV): -885.980851 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.042851 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.337900 | 1.038900 | 0.620200 |
| 2 | 6 | 0 | -3.900300 | 0.834500 | 2.069500 |
| 3 | 6 | 0 | -5.082300 | 1.070100 | 3.019200 |
| 4 | 6 | 0 | -5.735900 | 2.469600 | 2.826700 |

| | | | | | |
|---|---|---|---|---|---|
| 5 | 6 | 0 | -5.914800 | 2.860100 | 1.343100 |
| 6 | 6 | 0 | -4.807400 | 2.474300 | 0.362500 |
| 7 | 6 | 0 | -3.662300 | 3.476400 | 0.475700 |
| 8 | 6 | 0 | -4.723100 | 0.858500 | 4.475600 |
| 9 | 6 | 0 | -7.199500 | 2.427000 | 3.224700 |
| 10 | 6 | 0 | -7.937700 | 2.210900 | 2.059300 |
| 11 | 6 | 0 | -7.873400 | 2.474100 | 4.438600 |
| 12 | 6 | 0 | -9.266100 | 2.319300 | 4.447400 |
| 13 | 6 | 0 | -9.977900 | 2.097200 | 3.272200 |
| 14 | 6 | 0 | -9.306300 | 2.036400 | 2.041900 |
| 15 | 8 | 0 | -7.254200 | 2.689400 | 5.629800 |
| 16 | 8 | 0 | -7.139500 | 2.208000 | 0.944700 |
| 17 | 8 | 0 | -5.298700 | 2.603200 | -0.959600 |
| 18 | 6 | 0 | -11.477700 | 1.943000 | 3.304900 |
| 19 | 6 | 0 | -3.452400 | 1.497700 | 4.976900 |
| 20 | 6 | 0 | -5.513100 | 0.143100 | 5.281800 |
| 21 | 1 | 0 | -3.529000 | 0.811100 | -0.080900 |
| 22 | 1 | 0 | -5.169300 | 0.359700 | 0.390600 |
| 23 | 1 | 0 | -3.069100 | 1.508500 | 2.308400 |
| 24 | 1 | 0 | -3.526200 | -0.184600 | 2.216900 |
| 25 | 1 | 0 | -5.853400 | 0.335300 | 2.754400 |
| 26 | 1 | 0 | -5.160200 | 3.240400 | 3.352500 |
| 27 | 1 | 0 | -6.095000 | 3.942900 | 1.275700 |
| 28 | 1 | 0 | -2.843200 | 3.174800 | -0.181900 |
| 29 | 1 | 0 | -4.013600 | 4.460700 | 0.157900 |
| 30 | 1 | 0 | -3.281500 | 3.553900 | 1.497700 |
| 31 | 1 | 0 | -9.775400 | 2.365500 | 5.404300 |
| 32 | 1 | 0 | -9.837500 | 1.877800 | 1.109900 |
| 33 | 1 | 0 | -6.343400 | 2.371700 | 5.560800 |
| 34 | 1 | 0 | -6.153600 | 2.152700 | -0.986700 |
| 35 | 1 | 0 | -11.839200 | 1.787300 | 4.323100 |
| 36 | 1 | 0 | -11.967800 | 2.837000 | 2.906900 |
| 37 | 1 | 0 | -11.798200 | 1.095200 | 2.693100 |
| 38 | 1 | 0 | -3.382200 | 2.550100 | 4.678000 |
| 39 | 1 | 0 | -3.386000 | 1.444100 | 6.065600 |
| 40 | 1 | 0 | -2.574800 | 0.993100 | 4.559100 |
| 41 | 1 | 0 | -5.278000 | 0.003900 | 6.333300 |
| 42 | 1 | 0 | -6.422300 | -0.321900 | 4.911300 |

---

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 149.3241 Anisotropy = 23.2609

XX= 139.0885 YX= 0.2028 ZX= 4.1897

XY= 6.5478 YY= 158.3157 ZY= -6.5591

XZ= -1.4588 YZ= -12.3659 ZZ= 150.5680

Eigenvalues: 137.5678 145.5730 164.8314

2 C Isotropic = 157.3298 Anisotropy = 15.5712

XX= 158.4955 YX= 6.9959 ZX= 5.8864

XY= 4.0987 YY= 163.1002 ZY= -1.5984

```
XZ=     7.2253   YZ=     1.7259   ZZ=   150.3937
Eigenvalues:   146.2812   157.9976   167.7106
   3  C    Isotropic =   133.5740   Anisotropy =    13.9149
XX=   136.1288   YX=     1.2017   ZX=     2.1565
XY=    -7.3090   YY=   138.4727   ZY=     5.7760
XZ=     0.4425   YZ=     9.4449   ZZ=   126.1204
Eigenvalues:   122.0486   135.8227   142.8506
   4  C    Isotropic =   140.4911   Anisotropy =    21.9131
XX=   144.9325   YX=     1.5344   ZX=     2.6468
XY=     2.0908   YY=   149.0615   ZY=    -1.2295
XZ=     7.8616   YZ=   -24.5051   ZZ=   127.4794
Eigenvalues:   120.2392   146.1343   155.0998
   5  C    Isotropic =    95.1782   Anisotropy =    58.9468
XX=   119.1960   YX=    -5.4878   ZX=   -23.7772
XY=    -2.1528   YY=    88.2384   ZY=    25.5339
XZ=   -28.2618   YZ=     8.2102   ZZ=    78.1001
Eigenvalues:    58.9047    92.1537   134.4761
   6  C    Isotropic =   115.9770   Anisotropy =    48.9134
XX=    96.8248   YX=    -4.7467   ZX=    -1.3647
XY=     7.0581   YY=   147.3515   ZY=     5.8786
XZ=    -1.5202   YZ=     8.9013   ZZ=   103.7548
Eigenvalues:    96.3869   102.9583   148.5859
   7  C    Isotropic =   162.8845   Anisotropy =    39.0527
XX=   171.7223   YX=    -4.9375   ZX=   -16.2834
XY=    -4.1064   YY=   146.1289   ZY=     0.8553
XZ=   -18.2791   YZ=     1.2423   ZZ=   170.8022
Eigenvalues:   145.1140   154.6198   188.9196
   8  C    Isotropic =    28.5367   Anisotropy =   192.2129
XX=    55.8081   YX=    12.6726   ZX=    78.0603
XY=    19.5756   YY=   -51.1930   ZY=   -64.2157
XZ=    80.6387   YZ=   -65.5159   ZZ=    80.9950
Eigenvalues:   -93.6277    22.5591   156.6786
   9  C    Isotropic =    66.0091   Anisotropy =   109.2488
XX=    20.2683   YX=    -1.4795   ZX=     8.9404
XY=    12.6488   YY=    58.8892   ZY=   -36.6279
XZ=    21.9866   YZ=   -40.4816   ZZ=   118.8698
Eigenvalues:    13.8790    45.3067   138.8417
  10  C    Isotropic =    21.5533   Anisotropy =   110.5426
XX=   -25.0157   YX=   -37.7847   ZX=    -1.1425
XY=   -46.8389   YY=     2.6820   ZY=   -31.5989
XZ=   -10.4817   YZ=   -22.2665   ZZ=    86.9937
Eigenvalues:   -58.6513    28.0629    95.2484
  11  C    Isotropic =    28.0455   Anisotropy =   133.8140
XX=    15.9720   YX=    11.2461   ZX=    10.9278
XY=     6.0669   YY=   -26.3463   ZY=   -58.8657
XZ=     5.0835   YZ=   -54.9096   ZZ=    94.5110
Eigenvalues:   -50.7271    17.6089   117.2549
  12  C    Isotropic =    71.7932   Anisotropy =   116.6569
XX=    23.8337   YX=   -33.8625   ZX=    -4.6820
XY=   -45.8769   YY=    52.7487   ZY=   -35.9575
XZ=    -2.9836   YZ=   -26.3558   ZZ=   138.7973
Eigenvalues:    -7.2784    73.0936   149.5645
```

```
  13  C    Isotropic =    41.1624   Anisotropy =   194.5255
XX=   -44.5683   YX=    12.3244   ZX=    22.1840
XY=    15.6495   YY=    26.9605   ZY=   -62.6264
XZ=    29.1355   YZ=   -64.2649   ZZ=   141.0950
Eigenvalues:   -55.8509     8.4920   170.8460
  14  C    Isotropic =    80.6448   Anisotropy =   123.6616
XX=    73.1995   YX=    -5.1447   ZX=     6.5586
XY=    10.9877   YY=    26.6321   ZY=   -56.9772
XZ=     7.3429   YZ=   -49.0767   ZZ=   142.1027
Eigenvalues:     5.5680    73.2805   163.0859
  15  O    Isotropic =   206.1317   Anisotropy =    80.9961
XX=   153.8566   YX=    -3.0231   ZX=    -1.0340
XY=   -13.8122   YY=   206.3771   ZY=   -21.3394
XZ=    29.6629   YZ=    20.7053   ZZ=   258.1613
Eigenvalues:   150.6903   207.5756   260.1291
  16  O    Isotropic =   192.6242   Anisotropy =   105.4835
XX=   217.2589   YX=    60.6673   ZX=    33.2480
XY=    50.3759   YY=   166.5473   ZY=   -34.0171
XZ=    27.0213   YZ=    36.0757   ZZ=   194.0663
Eigenvalues:   127.0105   187.9155   262.9465
  17  O    Isotropic =   255.5476   Anisotropy =    52.8293
XX=   235.9309   YX=   -19.5398   ZX=   -17.9908
XY=   -13.1160   YY=   281.2941   ZY=     7.9134
XZ=   -27.0244   YZ=     3.0200   ZZ=   249.4178
Eigenvalues:   217.5564   258.3192   290.7671
  18  C    Isotropic =   163.9935   Anisotropy =    41.2375
XX=   187.5340   YX=    -5.3692   ZX=    -9.3405
XY=   -11.3678   YY=   157.1281   ZY=     8.2551
XZ=    -5.4093   YZ=     5.4777   ZZ=   147.3183
Eigenvalues:   143.5842   156.9111   191.4851
  19  C    Isotropic =   167.4263   Anisotropy =    26.7948
XX=   167.3627   YX=    -5.7726   ZX=    -9.9776
XY=    -9.1661   YY=   169.6025   ZY=    11.1304
XZ=    -8.7023   YZ=     8.6545   ZZ=   165.3136
Eigenvalues:   156.0109   160.9784   185.2895
  20  C    Isotropic =    65.4300   Anisotropy =   116.5361
XX=   101.6202   YX=    24.6473   ZX=    35.5050
XY=    20.4125   YY=    -6.1577   ZY=   -55.8731
XZ=    40.6627   YZ=   -48.9305   ZZ=   100.8274
Eigenvalues:   -36.8251    89.9943   143.1207
  21  H    Isotropic =    30.1089   Anisotropy =     8.5909
XX=    32.9161   YX=     2.4806   ZX=     3.5015
XY=     2.4647   YY=    28.9100   ZY=     0.2414
XZ=     3.8599   YZ=     0.7440   ZZ=    28.5006
Eigenvalues:    26.1248    28.3658    35.8361
  22  H    Isotropic =    30.0319   Anisotropy =     5.5791
XX=    28.1732   YX=     0.1747   ZX=    -0.6693
XY=    -0.7996   YY=    28.9933   ZY=     1.3496
XZ=     0.0706   YZ=     2.5262   ZZ=    32.9293
Eigenvalues:    27.9950    28.3495    33.7513
  23  H    Isotropic =    30.2019   Anisotropy =     5.7831
XX=    31.2180   YX=    -1.1380   ZX=    -2.2381
```

```
XY=    -1.3271   YY=    32.8253   ZY=     1.5386
XZ=    -1.5659   YZ=     0.9748   ZZ=    26.5625
Eigenvalues:    25.7948    30.7536    34.0574
  24  H    Isotropic =    30.3743   Anisotropy =     9.8073
XX=    29.0106   YX=    -0.7875   ZX=     4.3202
XY=    -1.1296   YY=    30.8372   ZY=    -3.8500
XZ=     5.1935   YZ=    -3.1274   ZZ=    31.2750
Eigenvalues:    24.8471    29.3631    36.9125
  25  H    Isotropic =    29.5933   Anisotropy =     2.3334
XX=    30.0015   YX=     1.5043   ZX=    -1.4694
XY=    -0.3818   YY=    28.7532   ZY=    -0.4649
XZ=     0.4071   YZ=    -1.7446   ZZ=    30.0252
Eigenvalues:    28.0860    29.5450    31.1489
  26  H    Isotropic =    28.7428   Anisotropy =     4.1254
XX=    27.3113   YX=    -0.7562   ZX=     0.5800
XY=     1.1055   YY=    29.5113   ZY=     2.1151
XZ=    -1.0163   YZ=     1.9521   ZZ=    29.4060
Eigenvalues:    27.0839    27.6516    31.4931
  27  H    Isotropic =    27.6162   Anisotropy =     5.5923
XX=    27.2170   YX=    -1.0854   ZX=    -1.7029
XY=     0.7140   YY=    26.4047   ZY=    -0.6267
XZ=    -3.4189   YZ=    -2.8325   ZZ=    29.2270
Eigenvalues:    24.6249    26.8793    31.3445
  28  H    Isotropic =    30.6540   Anisotropy =     9.8734
XX=    36.8187   YX=     1.7195   ZX=    -0.5520
XY=     1.1599   YY=    27.1859   ZY=    -0.3612
XZ=    -2.1435   YZ=    -0.3588   ZZ=    27.9573
Eigenvalues:    26.9438    27.7819    37.2362
  29  H    Isotropic =    30.6357   Anisotropy =     9.1637
XX=    28.6028   YX=     0.6495   ZX=    -2.1291
XY=     0.4100   YY=    28.8927   ZY=    -3.0675
XZ=    -1.8985   YZ=    -4.2461   ZZ=    34.4114
Eigenvalues:    26.9251    28.2370    36.7448
  30  H    Isotropic =    30.4079   Anisotropy =     6.4586
XX=    28.5512   YX=    -0.3326   ZX=    -3.3879
XY=     0.2122   YY=    32.7292   ZY=     1.8598
XZ=    -3.6769   YZ=     2.7387   ZZ=    29.9432
Eigenvalues:    25.3585    31.1516    34.7136
  31  H    Isotropic =    25.2207   Anisotropy =     6.7155
XX=    27.3252   YX=    -2.3116   ZX=    -1.1952
XY=    -2.3341   YY=    25.9580   ZY=     2.0463
XZ=    -0.9336   YZ=     2.2023   ZZ=    22.3788
Eigenvalues:    21.3908    24.5736    29.6977
  32  H    Isotropic =    25.2883   Anisotropy =     7.5290
XX=    30.2151   YX=    -0.0315   ZX=    -0.7793
XY=    -0.5855   YY=    24.0016   ZY=     1.1839
XZ=    -0.7074   YZ=     1.3963   ZZ=    21.6483
Eigenvalues:    21.0448    24.5125    30.3077
  33  H    Isotropic =    26.9158   Anisotropy =    18.3611
XX=    34.0833   YX=    -4.1435   ZX=     6.9983
XY=    -6.0269   YY=    27.8635   ZY=     0.4253
XZ=     7.2752   YZ=    -2.1080   ZZ=    18.8006
```

```
Eigenvalues:    15.8774    25.7135    39.1565
  34  H    Isotropic =    29.9813   Anisotropy =    15.8901
XX=    33.3611   YX=    -2.0326   ZX=    -6.7870
XY=    -3.1024   YY=    31.7848   ZY=     6.0034
XZ=    -7.0389   YZ=     6.0558   ZZ=    24.7980
Eigenvalues:    19.4555    29.9136    40.5747
  35  H    Isotropic =    29.8140   Anisotropy =     7.9203
XX=    33.9985   YX=     3.4298   ZX=    -0.7475
XY=     1.0955   YY=    30.2209   ZY=     1.3050
XZ=    -1.6390   YZ=     0.9959   ZZ=    25.2228
Eigenvalues:    24.6572    29.6907    35.0942
  36  H    Isotropic =    29.3222   Anisotropy =     8.9252
XX=    30.8573   YX=    -3.4840   ZX=     1.4887
XY=    -3.1985   YY=    30.3397   ZY=    -2.2120
XZ=     2.6912   YZ=    -3.1247   ZZ=    26.7696
Eigenvalues:    25.3211    27.3731    35.2723
  37  H    Isotropic =    29.4795   Anisotropy =     8.0885
XX=    30.1236   YX=    -1.7223   ZX=    -2.6441
XY=    -0.0810   YY=    27.4603   ZY=     3.6711
XZ=    -2.2196   YZ=     4.3647   ZZ=    30.8547
Eigenvalues:    24.7208    28.8459    34.8718
  38  H    Isotropic =    29.9193   Anisotropy =     4.5734
XX=    26.9240   YX=    -0.2140   ZX=    -2.0943
XY=    -1.0722   YY=    30.8039   ZY=     1.0949
XZ=    -2.3403   YZ=    -0.5434   ZZ=    32.0299
Eigenvalues:    26.0414    30.7482    32.9682
  39  H    Isotropic =    29.9516   Anisotropy =     8.3784
XX=    28.3504   YX=     0.2662   ZX=    -0.9197
XY=     1.5441   YY=    34.8552   ZY=     1.8404
XZ=    -0.2956   YZ=     2.7932   ZZ=    26.6492
Eigenvalues:    25.7751    28.5426    35.5372
  40  H    Isotropic =    29.8794   Anisotropy =     8.0652
XX=    33.4936   YX=    -2.1805   ZX=     1.7947
XY=    -2.9571   YY=    30.6121   ZY=     0.8525
XZ=     2.4219   YZ=     0.1997   ZZ=    25.5326
Eigenvalues:    24.7651    29.6169    35.2562
  41  H    Isotropic =    26.6094   Anisotropy =     5.7354
XX=    27.8841   YX=     3.3272   ZX=    -0.9679
XY=     0.4350   YY=    26.5648   ZY=    -1.5879
XZ=    -1.0851   YZ=    -3.6815   ZZ=    25.3791
Eigenvalues:    23.2349    26.1602    30.4330
  42  H    Isotropic =    26.6315   Anisotropy =     7.0518
XX=    27.1592   YX=     0.4471   ZX=    -1.1746
XY=     2.6816   YY=    25.7350   ZY=    -4.2662
XZ=    -0.4592   YZ=    -4.2669   ZZ=    27.0001
Eigenvalues:    21.9676    26.5941    31.3326
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 50.06 | 75.50 | 96.54 | 106.21 | 138.48 | 152.35 |
| intensities | 0.56 | 1.23 | 1.16 | 0.34 | 0.72 | 1.05 |
| reduc. mass | 1.12 | 0.94 | 1.05 | 1.84 | 0.29 | 1.31 |
| force const | 0.00 | 0.00 | 0.01 | 0.01 | 0.00 | 0.02 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 174.20 | 206.98 | 222.92 | 231.97 | 247.86 | 263.11 |
| intensities | 0.49 | 0.14 | 1.04 | 2.75 | 0.61 | 0.28 |
| reduc. mass | 0.72 | 0.68 | 1.12 | 0.42 | 0.53 | 0.82 |
| force const | 0.01 | 0.02 | 0.03 | 0.01 | 0.02 | 0.03 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 270.49 | 282.07 | 302.72 | 306.60 | 322.48 | 344.44 |
| intensities | 6.83 | 0.06 | 0.96 | 2.08 | 5.66 | 0.77 |
| reduc. mass | 0.98 | 1.06 | 0.66 | 0.91 | 0.47 | 0.83 |
| force const | 0.04 | 0.05 | 0.04 | 0.05 | 0.03 | 0.06 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 368.92 | 416.64 | 424.00 | 470.36 | 495.28 | 507.32 |
| intensities | 0.31 | 0.70 | 3.86 | 2.42 | 21.16 | 3.18 |
| reduc. mass | 1.18 | 0.99 | 0.61 | 0.54 | 1.01 | 0.66 |
| force const | 0.09 | 0.10 | 0.06 | 0.07 | 0.15 | 0.10 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 521.43 | 527.67 | 546.95 | 567.04 | 592.35 | 619.07 |
| intensities | 4.11 | 4.89 | 4.36 | 14.18 | 25.67 | 99.27 |
| reduc. mass | 1.45 | 0.79 | 0.64 | 0.55 | 2.10 | 0.71 |
| force const | 0.23 | 0.13 | 0.11 | 0.10 | 0.43 | 0.16 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 630.34 | 660.54 | 677.90 | 699.50 | 725.93 | 743.78 |
| intensities | 99.34 | 2.32 | 4.67 | 8.19 | 13.28 | 3.36 |
| reduc. mass | 0.71 | 0.75 | 0.74 | 0.54 | 0.38 | 0.42 |
| force const | 0.17 | 0.19 | 0.20 | 0.16 | 0.12 | 0.14 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 746.44 | 799.00 | 818.99 | 827.61 | 865.32 | 924.34 |
| intensities | 12.76 | 7.42 | 3.88 | 2.07 | 12.06 | 1.49 |
| reduc. mass | 1.00 | 0.55 | 0.86 | 1.78 | 0.52 | 0.69 |
| force const | 0.33 | 0.21 | 0.34 | 0.72 | 0.23 | 0.35 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 930.36 | 950.88 | 964.89 | 993.96 | 1011.09 | 1022.57 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 7.48 | 12.55 | 13.84 | 10.88 | 3.59 | 7.12 |
| reduc. mass | 0.69 | 1.23 | 0.27 | 0.36 | 0.27 | 0.20 |
| force const | 0.35 | 0.66 | 0.15 | 0.21 | 0.16 | 0.12 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1031.03 | 1040.56 | 1050.13 | 1058.90 | 1067.21 | 1090.29 |
| intensities | 27.89 | 18.60 | 3.76 | 23.10 | 33.89 | 28.40 |
| reduc. mass | 0.35 | 0.40 | 0.45 | 0.29 | 0.26 | 0.29 |
| force const | 0.22 | 0.25 | 0.29 | 0.19 | 0.17 | 0.21 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1099.05 | 1128.40 | 1132.17 | 1150.92 | 1162.60 | 1225.99 |
| intensities | 8.26 | 20.14 | 41.25 | 22.03 | 29.05 | 61.50 |
| reduc. mass | 0.43 | 0.37 | 0.35 | 0.48 | 0.69 | 0.66 |
| force const | 0.31 | 0.28 | 0.27 | 0.37 | 0.55 | 0.59 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1238.56 | 1248.02 | 1258.80 | 1298.93 | 1303.72 | 1340.53 |
| intensities | 30.80 | 43.64 | 56.12 | 95.57 | 78.75 | 74.52 |
| reduc. mass | 0.26 | 0.19 | 0.71 | 0.62 | 1.56 | 0.45 |
| force const | 0.23 | 0.18 | 0.66 | 0.61 | 1.56 | 0.47 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1346.78 | 1377.44 | 1398.48 | 1402.25 | 1410.72 | 1474.13 |
| intensities | 28.57 | 350.75 | 151.69 | 134.50 | 55.17 | 71.99 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.94 | 0.68 | 0.42 | 1.06 | 0.40 | 1.44 |
| force const | 1.00 | 0.76 | 0.48 | 1.23 | 0.47 | 1.85 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1487.21 | 1491.68 | 1508.23 | 1524.58 | 1535.91 | 1537.09 |
| intensities | 1.92 | 3.97 | 148.11 | 86.61 | 30.51 | 104.89 |
| reduc. mass | 0.81 | 0.67 | 1.07 | 0.65 | 0.82 | 0.94 |
| force const | 1.05 | 0.87 | 1.43 | 0.90 | 1.14 | 1.30 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1572.73 | 1580.31 | 1604.76 | 1622.92 | 1638.78 | 1647.65 |
| intensities | 18.72 | 34.64 | 7.93 | 16.84 | 66.78 | 97.14 |
| reduc. mass | 0.70 | 0.73 | 0.55 | 0.57 | 0.19 | 0.35 |
| force const | 1.02 | 1.07 | 0.84 | 0.89 | 0.30 | 0.56 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1655.05 | 1657.35 | 1659.68 | 1660.56 | 1664.89 | 1666.82 |
| intensities | 28.55 | 10.49 | 47.66 | 15.97 | 8.85 | 80.59 |
| reduc. mass | 0.17 | 0.17 | 0.20 | 0.17 | 0.17 | 0.15 |
| force const | 0.27 | 0.27 | 0.33 | 0.27 | 0.28 | 0.24 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1669.06 | 1676.81 | 1682.08 | 1693.38 | 1727.59 | 1802.77 |
| intensities | 4.45 | 61.31 | 40.12 | 7.61 | 35.53 | 743.99 |
| reduc. mass | 0.16 | 0.27 | 0.40 | 1.62 | 1.05 | 1.56 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 0.27 | 0.45 | 0.66 | 2.74 | 1.85 | 2.99 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1837.14 | 1889.55 | 3024.32 | 3028.70 | 3036.50 | 3053.58 |
| intensities | 421.20 | 9.37 | 523.52 | 192.92 | 655.27 | 421.63 |
| reduc. mass | 1.37 | 0.88 | 0.31 | 0.32 | 0.28 | 0.51 |
| force const | 2.73 | 1.84 | 1.65 | 1.71 | 1.51 | 2.81 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3063.28 | 3073.84 | 3086.79 | 3096.74 | 3104.40 | 3123.26 |
| intensities | 380.21 | 389.85 | 361.31 | 20.65 | 340.08 | 544.45 |
| reduc. mass | 0.44 | 0.85 | 0.43 | 0.44 | 0.38 | 0.43 |
| force const | 2.44 | 4.75 | 2.43 | 2.51 | 2.16 | 2.46 |

| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3126.90 | 3129.34 | 3137.92 | 3144.36 | 3146.91 | 3148.96 |
| intensities | 321.56 | 389.49 | 534.24 | 708.63 | 242.91 | 187.83 |
| reduc. mass | 0.34 | 0.31 | 0.50 | 0.28 | 0.21 | 0.18 |
| force const | 1.94 | 1.81 | 2.90 | 1.66 | 1.22 | 1.08 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3155.54 | 3164.04 | 3169.93 | 3197.74 | 3832.33 | 3842.21 |
| intensities | 334.82 | 612.28 | 200.52 | 277.08 | 60.83 | 20.90 |
| reduc. mass | 0.43 | 0.19 | 0.37 | 0.54 | 0.75 | 0.75 |
| force const | 2.51 | 1.14 | 2.17 | 3.23 | 6.48 | 6.52 |

Number of imaginary frequencies: 0

Conformation 6

Boltzmann Population = 50.1% (relative energy = 0.00 kcal/mol)

Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.982993 hartrees

Total enthalpy, Htot (Utot + pV): -885.982049 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.044439 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -4.335200 | 0.978100 | 0.622600 |
| 2 | 6 | 0 | -3.905600 | 0.812500 | 2.081200 |
| 3 | 6 | 0 | -5.102200 | 1.085300 | 3.000700 |

| | | | | | |
|---|---|---|---|---|---|
| 4 | 6 | 0 | -5.702500 | 2.495400 | 2.772700 |
| 5 | 6 | 0 | -5.901200 | 2.847600 | 1.286300 |
| 6 | 6 | 0 | -4.812000 | 2.402300 | 0.308000 |
| 7 | 6 | 0 | -3.659500 | 3.401200 | 0.360300 |
| 8 | 6 | 0 | -4.799800 | 0.867900 | 4.474700 |
| 9 | 6 | 0 | -7.150700 | 2.502200 | 3.208600 |
| 10 | 6 | 0 | -7.924400 | 2.271500 | 2.070300 |
| 11 | 6 | 0 | -7.769400 | 2.531600 | 4.450300 |
| 12 | 6 | 0 | -9.160300 | 2.370800 | 4.514700 |
| 13 | 6 | 0 | -9.913900 | 2.153100 | 3.364500 |
| 14 | 6 | 0 | -9.292200 | 2.093000 | 2.107100 |
| 15 | 8 | 0 | -7.094900 | 2.698200 | 5.616300 |
| 16 | 8 | 0 | -7.157200 | 2.228100 | 0.933600 |
| 17 | 8 | 0 | -5.319900 | 2.471300 | -1.012200 |
| 18 | 6 | 0 | -11.411600 | 2.002300 | 3.454800 |
| 19 | 6 | 0 | -5.578300 | -0.224100 | 5.153900 |
| 20 | 6 | 0 | -3.903500 | 1.618100 | 5.124600 |
| 21 | 1 | 0 | -3.523800 | 0.730100 | -0.068700 |
| 22 | 1 | 0 | -5.162000 | 0.286900 | 0.411700 |
| 23 | 1 | 0 | -3.076100 | 1.487200 | 2.325500 |
| 24 | 1 | 0 | -3.538700 | -0.203900 | 2.259300 |
| 25 | 1 | 0 | -5.885000 | 0.370600 | 2.711900 |
| 26 | 1 | 0 | -5.081000 | 3.252800 | 3.262100 |
| 27 | 1 | 0 | -6.046900 | 3.933500 | 1.190500 |
| 28 | 1 | 0 | -2.861400 | 3.075300 | -0.311100 |
| 29 | 1 | 0 | -4.011800 | 4.379700 | 0.025800 |
| 30 | 1 | 0 | -3.248900 | 3.501900 | 1.368600 |
| 31 | 1 | 0 | -9.634300 | 2.409400 | 5.489800 |
| 32 | 1 | 0 | -9.860200 | 1.922400 | 1.199400 |
| 33 | 1 | 0 | -6.142200 | 2.632100 | 5.452300 |
| 34 | 1 | 0 | -6.185000 | 2.040200 | -1.003800 |
| 35 | 1 | 0 | -11.729100 | 1.795200 | 4.478600 |
| 36 | 1 | 0 | -11.912700 | 2.918300 | 3.126400 |
| 37 | 1 | 0 | -11.763800 | 1.189300 | 2.813900 |
| 38 | 1 | 0 | -5.393400 | -1.183400 | 4.657400 |
| 39 | 1 | 0 | -5.315500 | -0.318800 | 6.209500 |
| 40 | 1 | 0 | -6.653500 | -0.024800 | 5.075000 |
| 41 | 1 | 0 | -3.683700 | 1.453700 | 6.175100 |
| 42 | 1 | 0 | -3.341000 | 2.402200 | 4.623200 |

---

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 147.7946 Anisotropy = 23.8393

XX= 137.4911 YX= -2.1634 ZX= 3.5091

XY= -9.3983 YY= 158.2548 ZY= 5.1477

XZ= -2.1026 YZ= 11.4894 ZZ= 147.6380

Eigenvalues: 135.2142 144.4822 163.6875

2 C Isotropic = 153.6816 Anisotropy = 23.9990

XX= 160.6428 YX= -9.2204 ZX= 5.0834

```
XY=    -3.4302   YY=   159.9996   ZY=    -5.8538
XZ=     6.3517   YZ=    -9.3676   ZZ=   140.4024
Eigenvalues:   137.2561   154.1078   169.6809
   3  C    Isotropic =   135.4618   Anisotropy =    11.6756
XX=   141.2334   YX=    -3.8478   ZX=    -0.5567
XY=     8.9823   YY=   139.8462   ZY=    -2.8036
XZ=     6.4617   YZ=    -7.3269   ZZ=   125.3058
Eigenvalues:   123.0047   140.1352   143.2455
   4  C    Isotropic =   134.4419   Anisotropy =    30.0952
XX=   124.1812   YX=     4.5957   ZX=     2.3902
XY=     1.2142   YY=   151.7798   ZY=    -3.1581
XZ=     8.8468   YZ=    18.0656   ZZ=   127.3647
Eigenvalues:   119.7577   129.0626   154.5053
   5  C    Isotropic =    95.3805   Anisotropy =    58.0435
XX=   118.8134   YX=     7.6187   ZX=   -19.9392
XY=     4.2612   YY=    87.3125   ZY=   -27.8672
XZ=   -26.6754   YZ=   -11.2965   ZZ=    80.0157
Eigenvalues:    59.7821    92.2833   134.0762
   6  C    Isotropic =   115.9626   Anisotropy =    48.4884
XX=    97.3456   YX=    -1.1849   ZX=    -0.5468
XY=   -12.0995   YY=   144.9634   ZY=    -8.4603
XZ=     0.2529   YZ=   -12.0731   ZZ=   105.5789
Eigenvalues:    96.1165   103.4832   148.2882
   7  C    Isotropic =   162.3200   Anisotropy =    40.1642
XX=   170.9539   YX=     6.3254   ZX=   -16.4951
XY=     5.9022   YY=   145.1167   ZY=    -0.8837
XZ=   -18.7018   YZ=    -1.0559   ZZ=   170.8893
Eigenvalues:   143.2515   154.6123   189.0961
   8  C    Isotropic =    17.3031   Anisotropy =   211.8557
XX=    46.5089   YX=    79.8599   ZX=   100.2711
XY=    82.1188   YY=   -31.7469   ZY=    -6.7871
XZ=    96.1881   YZ=     1.0829   ZZ=    37.1474
Eigenvalues:  -108.8298     2.1989   158.5403
   9  C    Isotropic =    67.8916   Anisotropy =   106.9999
XX=    23.8729   YX=    -1.4756   ZX=     8.5404
XY=   -15.9881   YY=    60.7777   ZY=    37.8787
XZ=    15.4709   YZ=    40.7282   ZZ=   119.0240
Eigenvalues:    16.4072    48.0426   139.2248
  10  C    Isotropic =    21.5991   Anisotropy =   109.6759
XX=   -30.5417   YX=    34.4098   ZX=    -5.5523
XY=    44.4481   YY=    12.1454   ZY=    35.8715
XZ=   -16.7739   YZ=    25.5122   ZZ=    83.1935
Eigenvalues:   -58.6928    28.7736    94.7164
  11  C    Isotropic =    28.4147   Anisotropy =   135.0790
XX=    14.9521   YX=    -6.3432   ZX=     9.9553
XY=    -0.4144   YY=   -25.2141   ZY=    60.8580
XZ=     6.5692   YZ=    52.8517   ZZ=    95.5062
Eigenvalues:   -48.3815    15.1583   118.4674
  12  C    Isotropic =    73.8265   Anisotropy =   116.6887
XX=    20.8820   YX=    30.9184   ZX=    -4.2809
XY=    42.1476   YY=    60.6812   ZY=    37.3506
XZ=    -5.9101   YZ=    26.4465   ZZ=   139.9164
```

```
Eigenvalues:    -3.9450    73.8056   151.6190
  13  C    Isotropic =    40.9411   Anisotropy =   194.2865
XX=   -42.1601   YX=   -15.1181   ZX=    21.3010
XY=   -17.8614   YY=    29.3688   ZY=    66.6505
XZ=    28.9436   YZ=    70.7790   ZZ=   135.6146
Eigenvalues:   -56.1280     8.4858   170.4655
  14  C    Isotropic =    81.2125   Anisotropy =   122.5971
XX=    73.9830   YX=     9.5172   ZX=     2.8571
XY=    -7.5666   YY=    32.7681   ZY=    60.8103
XZ=     4.3480   YZ=    55.2621   ZZ=   136.8864
Eigenvalues:     6.8585    73.8351   162.9439
  15  O    Isotropic =   203.2016   Anisotropy =    76.2474
XX=   148.1229   YX=    13.6720   ZX=     0.0256
XY=     6.0790   YY=   210.3827   ZY=    10.9373
XZ=    23.5218   YZ=   -29.7993   ZZ=   251.0992
Eigenvalues:   144.9696   210.6021   254.0332
  16  O    Isotropic =   193.1758   Anisotropy =   104.6400
XX=   225.0035   YX=   -54.5162   ZX=    34.4980
XY=   -48.1269   YY=   159.9280   ZY=    36.5025
XZ=    26.4214   YZ=   -30.8425   ZZ=   194.5959
Eigenvalues:   126.9897   189.6019   262.9358
  17  O    Isotropic =   257.0632   Anisotropy =    53.2051
XX=   236.8251   YX=    14.3043   ZX=   -19.6587
XY=     7.8377   YY=   282.7798   ZY=   -11.8610
XZ=   -28.6909   YZ=    -8.8657   ZZ=   251.5846
Eigenvalues:   218.8035   259.8528   292.5333
  18  C    Isotropic =   163.7609   Anisotropy =    41.4816
XX=   185.8938   YX=     7.1304   ZX=   -10.1712
XY=    12.8805   YY=   157.8998   ZY=    -9.5690
XZ=    -5.8368   YZ=    -6.0240   ZZ=   147.4892
Eigenvalues:   143.1606   156.7068   191.4153
  19  C    Isotropic =   158.0418   Anisotropy =    42.4420
XX=   158.3359   YX=   -15.2407   ZX=   -17.0571
XY=   -12.0332   YY=   160.7164   ZY=     9.2358
XZ=   -18.6129   YZ=    12.2630   ZZ=   155.0729
Eigenvalues:   138.6801   149.1087   186.3364
  20  C    Isotropic =    72.5081   Anisotropy =   130.2649
XX=    92.5426   YX=    75.2917   ZX=    47.6763
XY=    71.5125   YY=    22.0723   ZY=   -16.6159
XZ=    48.5968   YZ=   -18.9510   ZZ=   102.9094
Eigenvalues:   -36.4851    94.6581   159.3514
  21  H    Isotropic =    30.0618   Anisotropy =     8.4269
XX=    33.3182   YX=    -1.8787   ZX=     3.4555
XY=    -1.8416   YY=    28.2912   ZY=     0.3698
XZ=     3.9367   YZ=    -0.1370   ZZ=    28.5760
Eigenvalues:    26.0539    28.4518    35.6798
  22  H    Isotropic =    30.1232   Anisotropy =     5.5432
XX=    27.9654   YX=    -0.7056   ZX=    -0.4297
XY=     0.5088   YY=    29.0693   ZY=    -1.0039
XZ=     0.3465   YZ=    -2.0272   ZZ=    33.3351
Eigenvalues:    27.9476    28.6034    33.8187
  23  H    Isotropic =    30.3843   Anisotropy =     5.6469
```

```
XX=    31.4831   YX=     1.1193   ZX=    -2.4294
XY=     1.8426   YY=    32.1326   ZY=    -1.8278
XZ=    -1.4454   YZ=    -1.0039   ZZ=    27.5373
Eigenvalues:    26.6293    30.3748    34.1489
  24  H    Isotropic =    30.1583   Anisotropy =     9.1936
XX=    29.4865   YX=     0.2942   ZX=     3.6620
XY=     0.9344   YY=    30.8970   ZY=     4.6826
XZ=     4.0911   YZ=     3.8403   ZZ=    30.0912
Eigenvalues:    24.6665    29.5209    36.2873
  25  H    Isotropic =    30.0490   Anisotropy =     3.6932
XX=    30.6377   YX=    -1.5216   ZX=    -2.3433
XY=    -0.2699   YY=    29.8435   ZY=     0.7256
XZ=     0.2118   YZ=     2.7336   ZZ=    29.6658
Eigenvalues:    28.0111    29.6248    32.5111
  26  H    Isotropic =    28.7747   Anisotropy =     4.3624
XX=    27.6366   YX=    -0.1081   ZX=     0.1224
XY=    -1.7304   YY=    29.4525   ZY=    -2.1764
XZ=    -1.1195   YZ=    -2.4432   ZZ=    29.2350
Eigenvalues:    26.2870    28.3542    31.6830
  27  H    Isotropic =    27.6120   Anisotropy =     5.7526
XX=    27.4320   YX=     1.1300   ZX=    -1.8107
XY=    -0.7280   YY=    26.3794   ZY=     0.5678
XZ=    -3.8378   YZ=     2.6847   ZZ=    29.0245
Eigenvalues:    24.5096    26.8793    31.4470
  28  H    Isotropic =    30.6299   Anisotropy =     9.8871
XX=    37.0015   YX=    -0.9504   ZX=    -0.4734
XY=    -0.3644   YY=    26.9370   ZY=     0.3773
XZ=    -2.0572   YZ=     0.1853   ZZ=    27.9513
Eigenvalues:    26.8522    27.8162    37.2213
  29  H    Isotropic =    30.6169   Anisotropy =     9.0566
XX=    28.8010   YX=    -0.7805   ZX=    -2.3344
XY=    -0.5269   YY=    29.0337   ZY=     3.0878
XZ=    -2.1836   YZ=     4.2948   ZZ=    34.0159
Eigenvalues:    26.8952    28.3009    36.6546
  30  H    Isotropic =    30.2951   Anisotropy =     6.6388
XX=    28.6818   YX=    -0.0239   ZX=    -3.2891
XY=    -0.5027   YY=    32.0944   ZY=    -2.3992
XZ=    -3.3643   YZ=    -3.2828   ZZ=    30.1091
Eigenvalues:    25.3520    30.8123    34.7210
  31  H    Isotropic =    25.2290   Anisotropy =     6.7272
XX=    27.0765   YX=     2.3195   ZX=    -0.9989
XY=     2.5388   YY=    26.1605   ZY=    -2.2374
XZ=    -0.7397   YZ=    -2.2215   ZZ=    22.4502
Eigenvalues:    21.3919    24.5814    29.7139
  32  H    Isotropic =    25.3466   Anisotropy =     7.3788
XX=    30.0860   YX=     0.4617   ZX=    -0.7744
XY=     0.9596   YY=    24.1613   ZY=    -1.3087
XZ=    -0.6698   YZ=    -1.5582   ZZ=    21.7926
Eigenvalues:    21.1035    24.6705    30.2659
  33  H    Isotropic =    26.5190   Anisotropy =    16.8640
XX=    35.3683   YX=     4.1308   ZX=     3.3218
XY=     5.9215   YY=    26.2164   ZY=    -2.8137
```

```
XZ=     2.0940   YZ=    -0.4198   ZZ=    17.9724
Eigenvalues:    16.8810    24.9144    37.7617
  34  H    Isotropic =    30.0323   Anisotropy =    15.8805
XX=    33.2796   YX=     1.9305   ZX=    -6.1675
XY=     2.9587   YY=    31.3969   ZY=    -6.9024
XZ=    -6.4338   YZ=    -7.0464   ZZ=    25.4203
Eigenvalues:    19.5338    29.9437    40.6193
  35  H    Isotropic =    29.7988   Anisotropy =     7.9055
XX=    34.1445   YX=    -3.1925   ZX=    -0.9384
XY=    -0.9157   YY=    29.9155   ZY=    -1.2923
XZ=    -1.9837   YZ=    -1.0117   ZZ=    25.3364
Eigenvalues:    24.6627    29.6645    35.0691
  36  H    Isotropic =    29.3083   Anisotropy =     9.0487
XX=    30.5442   YX=     3.5675   ZX=     1.4005
XY=     3.4602   YY=    30.5993   ZY=     2.1526
XZ=     2.5963   YZ=     3.1041   ZZ=    26.7815
Eigenvalues:    25.4289    27.1553    35.3408
  37  H    Isotropic =    29.5037   Anisotropy =     8.0060
XX=    30.0053   YX=     1.8414   ZX=    -2.3558
XY=     0.1683   YY=    27.6784   ZY=    -3.9313
XZ=    -1.7585   YZ=    -4.5573   ZZ=    30.8273
Eigenvalues:    24.7001    28.9699    34.8410
  38  H    Isotropic =    30.0314   Anisotropy =     7.9515
XX=    27.3157   YX=    -0.7705   ZX=     0.7132
XY=    -1.1013   YY=    28.4526   ZY=     2.7581
XZ=     1.1644   YZ=     2.3887   ZZ=    34.3259
Eigenvalues:    26.1729    28.5889    35.3324
  39  H    Isotropic =    29.9725   Anisotropy =     8.7928
XX=    28.0067   YX=    -3.5755   ZX=    -0.7456
XY=    -2.0176   YY=    34.5121   ZY=    -0.1252
XZ=    -1.3374   YZ=     2.6557   ZZ=    27.3987
Eigenvalues:    26.5087    27.5744    35.8344
  40  H    Isotropic =    29.9753   Anisotropy =     5.6212
XX=    32.4029   YX=     2.3052   ZX=    -1.3418
XY=     1.7249   YY=    29.9960   ZY=     2.3203
XZ=    -0.2189   YZ=     3.9239   ZZ=    27.5268
Eigenvalues:    24.9664    31.2367    33.7227
  41  H    Isotropic =    26.3582   Anisotropy =     5.4842
XX=    25.3649   YX=     3.0799   ZX=    -1.1895
XY=     1.1251   YY=    27.4084   ZY=    -1.2237
XZ=    -0.0132   YZ=    -3.1383   ZZ=    26.3014
Eigenvalues:    23.7819    25.2784    30.0144
  42  H    Isotropic =    26.4264   Anisotropy =     8.0883
XX=    25.1061   YX=     0.6565   ZX=     0.2749
XY=     3.4699   YY=    28.3097   ZY=    -5.9680
XZ=    -0.8763   YZ=    -2.1130   ZZ=    25.8635
Eigenvalues:    22.4383    25.0223    31.8186
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 54.26 | 75.85 | 93.00 | 98.14 | 109.60 | 127.02 |
| intensities | 0.35 | 0.90 | 1.23 | 0.15 | 0.06 | 4.68 |
| reduc. mass | 1.37 | 0.91 | 0.36 | 0.72 | 1.80 | 1.64 |
| force const | 0.00 | 0.00 | 0.00 | 0.00 | 0.01 | 0.02 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 172.62 | 200.93 | 215.94 | 235.73 | 253.27 | 263.12 |
| intensities | 1.13 | 2.01 | 0.55 | 0.39 | 2.65 | 3.48 |
| reduc. mass | 0.83 | 0.66 | 1.20 | 0.61 | 0.79 | 0.96 |
| force const | 0.01 | 0.02 | 0.03 | 0.02 | 0.03 | 0.04 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 276.67 | 293.67 | 303.59 | 304.57 | 314.29 | 345.56 |
| intensities | 3.13 | 0.27 | 1.05 | 2.17 | 5.03 | 6.38 |
| reduc. mass | 1.23 | 0.17 | 0.79 | 0.29 | 0.64 | 0.85 |
| force const | 0.06 | 0.01 | 0.04 | 0.02 | 0.04 | 0.06 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 373.60 | 403.90 | 420.98 | 459.82 | 491.96 | 504.86 |
| intensities | 1.61 | 5.65 | 4.26 | 4.61 | 10.50 | 3.01 |
| reduc. mass | 1.00 | 0.86 | 0.65 | 0.61 | 1.34 | 0.59 |
| force const | 0.08 | 0.08 | 0.07 | 0.08 | 0.19 | 0.09 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 516.17 | 528.07 | 547.94 | 567.64 | 598.68 | 622.98 |
| intensities | 9.35 | 10.55 | 4.95 | 11.20 | 26.43 | 95.52 |
| reduc. mass | 0.76 | 1.21 | 0.63 | 0.58 | 1.96 | 0.86 |
| force const | 0.12 | 0.20 | 0.11 | 0.11 | 0.41 | 0.20 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 647.89 | 663.59 | 699.34 | 712.26 | 718.09 | 738.90 |
| intensities | 95.51 | 3.01 | 4.44 | 15.63 | 0.64 | 4.72 |
| reduc. mass | 0.74 | 1.08 | 0.94 | 0.99 | 0.34 | 0.79 |
| force const | 0.18 | 0.28 | 0.27 | 0.29 | 0.10 | 0.25 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 752.88 | 800.84 | 836.36 | 847.61 | 858.68 | 926.11 |
| intensities | 17.65 | 2.49 | 2.00 | 2.77 | 7.17 | 0.30 |
| reduc. mass | 0.74 | 1.27 | 2.11 | 0.78 | 0.70 | 0.72 |
| force const | 0.25 | 0.48 | 0.87 | 0.33 | 0.30 | 0.37 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 933.55 | 941.68 | 960.11 | 988.76 | 1014.54 | 1022.53 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 1.99 | 4.23 | 24.38 | 3.04 | 1.60 | 10.62 |
| reduc. mass | 0.53 | 0.60 | 0.34 | 0.26 | 0.26 | 0.24 |
| force const | 0.27 | 0.31 | 0.18 | 0.15 | 0.16 | 0.15 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1031.06 | 1038.26 | 1051.15 | 1055.10 | 1064.24 | 1088.86 |
| intensities | 29.69 | 14.58 | 9.89 | 2.97 | 45.97 | 40.06 |
| reduc. mass | 0.44 | 0.33 | 0.26 | 0.26 | 0.69 | 0.26 |
| force const | 0.28 | 0.21 | 0.17 | 0.17 | 0.46 | 0.18 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1098.59 | 1131.62 | 1134.33 | 1138.91 | 1161.89 | 1223.93 |
| intensities | 4.90 | 25.02 | 12.63 | 40.28 | 27.44 | 78.91 |
| reduc. mass | 0.52 | 0.46 | 0.60 | 0.67 | 0.74 | 0.68 |
| force const | 0.37 | 0.34 | 0.45 | 0.51 | 0.58 | 0.60 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1243.76 | 1251.13 | 1256.11 | 1294.51 | 1306.54 | 1307.22 |
| intensities | 13.36 | 102.87 | 22.29 | 23.24 | 135.13 | 108.74 |
| reduc. mass | 0.24 | 0.45 | 0.30 | 1.24 | 0.62 | 0.55 |
| force const | 0.22 | 0.42 | 0.28 | 1.22 | 0.62 | 0.55 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1347.24 | 1378.82 | 1402.27 | 1409.40 | 1435.42 | 1473.79 |
| intensities | 62.99 | 255.81 | 260.08 | 72.52 | 51.91 | 115.10 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.69 | 0.57 | 0.35 | 0.62 | 0.63 | 1.73 |
| force const | 0.73 | 0.64 | 0.40 | 0.73 | 0.77 | 2.22 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1494.69 | 1507.18 | 1510.48 | 1519.73 | 1521.90 | 1545.58 |
| intensities | 7.99 | 92.64 | 14.37 | 118.11 | 79.50 | 5.33 |
| reduc. mass | 0.50 | 0.55 | 1.02 | 0.79 | 0.56 | 2.02 |
| force const | 0.66 | 0.73 | 1.37 | 1.07 | 0.77 | 2.85 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1562.31 | 1571.41 | 1592.22 | 1624.92 | 1634.43 | 1640.60 |
| intensities | 63.51 | 20.18 | 7.40 | 22.41 | 19.67 | 19.98 |
| reduc. mass | 0.52 | 0.45 | 0.42 | 0.61 | 0.46 | 0.33 |
| force const | 0.74 | 0.66 | 0.63 | 0.95 | 0.72 | 0.52 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1651.00 | 1655.93 | 1659.77 | 1660.50 | 1663.69 | 1665.02 |
| intensities | 42.91 | 31.69 | 36.92 | 28.39 | 123.39 | 14.18 |
| reduc. mass | 0.19 | 0.23 | 0.15 | 0.22 | 0.31 | 0.24 |
| force const | 0.31 | 0.37 | 0.25 | 0.36 | 0.51 | 0.40 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1668.03 | 1670.73 | 1672.71 | 1686.02 | 1690.73 | 1802.79 |
| intensities | 11.79 | 6.31 | 20.24 | 42.88 | 64.07 | 842.11 |
| reduc. mass | 0.25 | 0.13 | 0.24 | 0.38 | 0.24 | 1.60 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 0.41 | 0.21 | 0.39 | 0.64 | 0.40 | 3.06 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1832.60 | 1888.91 | 3019.69 | 3034.42 | 3052.40 | 3060.15 |
| intensities | 452.88 | 17.34 | 295.46 | 334.35 | 403.69 | 673.14 |
| reduc. mass | 1.43 | 0.87 | 0.32 | 0.30 | 0.49 | 0.43 |
| force const | 2.83 | 1.82 | 1.73 | 1.60 | 2.68 | 2.36 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3074.52 | 3077.21 | 3091.48 | 3097.78 | 3118.23 | 3124.07 |
| intensities | 386.23 | 145.44 | 865.66 | 3.23 | 460.44 | 482.63 |
| reduc. mass | 0.84 | 0.75 | 0.29 | 0.77 | 0.14 | 0.27 |
| force const | 4.67 | 4.19 | 1.63 | 4.35 | 0.80 | 1.57 |

| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3125.82 | 3129.93 | 3136.16 | 3145.29 | 3147.71 | 3150.41 |
| intensities | 6.51 | 367.00 | 358.67 | 799.95 | 9.36 | 246.67 |
| reduc. mass | 0.17 | 0.12 | 0.46 | 0.22 | 0.34 | 0.20 |
| force const | 0.97 | 0.68 | 2.69 | 1.26 | 1.99 | 1.17 |

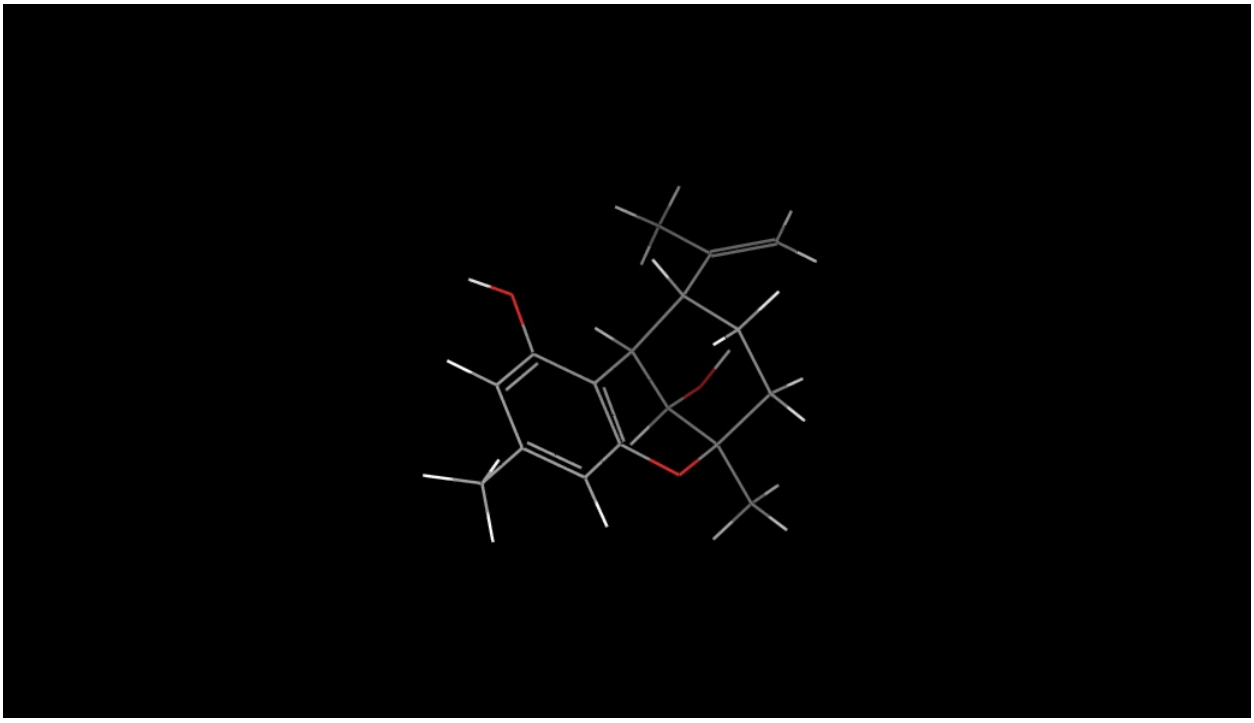
| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3158.39 | 3172.98 | 3189.42 | 3199.17 | 3824.96 | 3842.72 |
| intensities | 346.72 | 651.65 | 31.85 | 409.32 | 80.30 | 19.01 |
| reduc. mass | 0.44 | 0.23 | 0.15 | 0.27 | 0.94 | 0.94 |
| force const | 2.57 | 1.35 | 0.87 | 1.62 | 8.07 | 8.15 |

Number of imaginary frequencies: 0

5. DFT calculation data for the 6-membered cyclic ether (**9**). Energies, optimized geometries, NMR shielding values and IR frequencies from calculations performed at the mPW1PW91/6-311+G(2d,p)//M06-2X-D3/6-31G(d,p) level.

Conformation 1

Boltzmann Population = 47.0% (relative energy = 0.03 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.988043 hartrees

Total enthalpy, Htot (Utot + pV): -885.987099 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.047760 hartrees

```
 Geometry Optimization:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
```

| | | | | | |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.414200 | -1.941000 | 4.789100 |
| 2 | 6 | 0 | -1.081600 | -1.863400 | 3.292700 |
| 3 | 6 | 0 | -2.282000 | -1.451300 | 2.426500 |
| 4 | 6 | 0 | -2.929000 | -0.166200 | 3.024200 |
| 5 | 6 | 0 | -3.363700 | -0.371500 | 4.478400 |
| 6 | 6 | 0 | -2.113000 | -0.680400 | 5.320800 |
| 7 | 6 | 0 | -2.462000 | -0.822600 | 6.791700 |
| 8 | 6 | 0 | -3.302600 | -2.546400 | 2.154500 |
| 9 | 6 | 0 | -1.933900 | 0.963000 | 3.017300 |
| 10 | 6 | 0 | -1.131500 | 1.200100 | 4.133400 |
| 11 | 8 | 0 | -1.200200 | 0.436200 | 5.256900 |
| 12 | 6 | 0 | -1.759800 | 1.786500 | 1.902000 |
| 13 | 6 | 0 | -0.838900 | 2.827700 | 1.904000 |
| 14 | 6 | 0 | -0.053500 | 3.060500 | 3.037100 |
| 15 | 6 | 0 | -0.203200 | 2.244400 | 4.151200 |
| 16 | 6 | 0 | 0.973700 | 4.164200 | 3.028600 |
| 17 | 8 | 0 | -2.540300 | 1.502000 | 0.817700 |
| 18 | 6 | 0 | -3.161200 | -3.814600 | 2.554100 |
| 19 | 6 | 0 | -4.515700 | -2.117200 | 1.365400 |
| 20 | 8 | 0 | -4.362800 | -1.353600 | 4.644600 |
| 21 | 1 | 0 | -0.499400 | -2.094200 | 5.370800 |
| 22 | 1 | 0 | -2.067100 | -2.797300 | 4.998200 |
| 23 | 1 | 0 | -0.288000 | -1.123800 | 3.149100 |
| 24 | 1 | 0 | -0.673100 | -2.817100 | 2.945100 |
| 25 | 1 | 0 | -1.906400 | -1.154200 | 1.436100 |
| 26 | 1 | 0 | -3.794800 | 0.125300 | 2.423800 |
| 27 | 1 | 0 | -3.799400 | 0.562800 | 4.853000 |
| 28 | 1 | 0 | -1.561100 | -1.034000 | 7.373900 |
| 29 | 1 | 0 | -2.903300 | 0.107600 | 7.158700 |
| 30 | 1 | 0 | -3.183100 | -1.630200 | 6.927000 |
| 31 | 1 | 0 | -0.727600 | 3.457400 | 1.023900 |
| 32 | 1 | 0 | 0.392200 | 2.393200 | 5.045600 |
| 33 | 1 | 0 | 1.916900 | 3.812900 | 2.597100 |
| 34 | 1 | 0 | 0.635300 | 5.015600 | 2.432800 |
| 35 | 1 | 0 | 1.183000 | 4.515700 | 4.041200 |
| 36 | 1 | 0 | -2.356500 | 2.142600 | 0.121700 |
| 37 | 1 | 0 | -3.904400 | -4.563000 | 2.296200 |
| 38 | 1 | 0 | -2.308800 | -4.156500 | 3.131200 |
| 39 | 1 | 0 | -5.214700 | -1.574800 | 2.010800 |
| 40 | 1 | 0 | -4.232900 | -1.440500 | 0.551700 |
| 41 | 1 | 0 | -5.037500 | -2.978400 | 0.943900 |
| 42 | 1 | 0 | -4.074500 | -2.171900 | 4.216700 |

SCF GIAO Magnetic shielding tensor (ppm):
1 C Isotropic = 155.2155 Anisotropy = 30.0358
XX= 146.2589 YX= 4.9428 ZX= -7.7085
XY= 3.3253 YY= 156.2760 ZY= -7.8550

```
XZ=   -13.7477   YZ=   -13.5679   ZZ=   163.1117
Eigenvalues:   140.9552   149.4520   175.2394
   2  C    Isotropic =   165.1065   Anisotropy =    13.9819
XX=   156.5403   YX=    -0.5688   ZX=    -2.4859
XY=    -1.2914   YY=   174.1468   ZY=     2.3080
XZ=     0.1010   YZ=     0.5744   ZZ=   164.6325
Eigenvalues:   156.3390   164.5527   174.4278
   3  C    Isotropic =   140.7393   Anisotropy =    21.2607
XX=   151.7808   YX=     9.9485   ZX=    13.0989
XY=     3.9037   YY=   138.6888   ZY=    -2.0800
XZ=    -6.0748   YZ=    -5.0883   ZZ=   131.7482
Eigenvalues:   128.5575   138.7472   154.9131
   4  C    Isotropic =   149.7882   Anisotropy =    19.7756
XX=   150.5584   YX=     2.1057   ZX=    -1.4544
XY=    -3.2898   YY=   137.7229   ZY=    -8.1565
XZ=     2.5591   YZ=    -5.5043   ZZ=   161.0832
Eigenvalues:   135.8600   150.5327   162.9719
   5  C    Isotropic =   111.2472   Anisotropy =    45.9169
XX=   141.2799   YX=     8.4683   ZX=     4.7491
XY=     0.8897   YY=   102.1200   ZY=    -3.3733
XZ=    -6.4301   YZ=    -2.5700   ZZ=    90.3417
Eigenvalues:    89.6330   102.2501   141.8585
   6  C    Isotropic =   107.8425   Anisotropy =    63.8472
XX=   146.9141   YX=    -0.8820   ZX=    12.1283
XY=     8.6075   YY=    84.4381   ZY=    -4.8824
XZ=    16.0231   YZ=    -6.9165   ZZ=    92.1753
Eigenvalues:    79.5646    93.5557   150.4073
   7  C    Isotropic =   160.3740   Anisotropy =    41.9627
XX=   147.7121   YX=    -8.3757   ZX=     0.2735
XY=    -8.0720   YY=   177.3550   ZY=   -19.1945
XZ=    -0.3347   YZ=   -15.5339   ZZ=   156.0550
Eigenvalues:   142.4042   150.3687   188.3492
   8  C    Isotropic =    25.1790   Anisotropy =   197.2460
XX=   -17.0302   YX=   -50.9089   ZX=   -23.5094
XY=   -49.9470   YY=    32.8566   ZY=  -113.7090
XZ=   -26.8121   YZ=  -102.7792   ZZ=    59.7105
Eigenvalues:   -99.2268    18.0875   156.6763
   9  C    Isotropic =    73.2697   Anisotropy =   127.9567
XX=    26.9431   YX=    -0.3215   ZX=   -23.9379
XY=     2.0815   YY=    40.2408   ZY=   -20.3566
XZ=   -18.0377   YZ=   -14.4604   ZZ=   152.6252
Eigenvalues:    23.2789    37.9560   158.5742
  10  C    Isotropic =    24.5134   Anisotropy =   139.0053
XX=   -12.5501   YX=    38.2234   ZX=   -14.4236
XY=    45.1774   YY=   -24.5922   ZY=   -18.0855
XZ=   -15.3210   YZ=   -21.9800   ZZ=   110.6825
Eigenvalues:   -60.8818    17.2384   117.1836
  11  O    Isotropic =   170.3620   Anisotropy =    68.4607
XX=   123.1279   YX=    -2.1644   ZX=   -18.1205
XY=   -30.2642   YY=   181.8887   ZY=    -4.1087
XZ=   -13.5753   YZ=   -31.5008   ZZ=   206.0694
Eigenvalues:   114.5531   180.5304   216.0025
```

```
  12  C    Isotropic =    29.2696   Anisotropy =   130.0753
XX=    20.7652   YX=   -27.6130   ZX=   -19.5199
XY=   -18.3512   YY=   -43.3536   ZY=   -24.3242
XZ=   -15.5167   YZ=   -22.2865   ZZ=   110.3971
Eigenvalues:   -55.3491    27.1713   115.9864
  13  C    Isotropic =    80.3555   Anisotropy =    98.7018
XX=    63.4146   YX=    38.1766   ZX=    -8.9436
XY=    45.5579   YY=    36.1188   ZY=    -8.9237
XZ=   -14.3642   YZ=   -11.8393   ZZ=   141.5330
Eigenvalues:     5.7129    89.1968   146.1566
  14  C    Isotropic =    43.1925   Anisotropy =   193.5513
XX=   -47.1964   YX=    -8.4736   ZX=   -39.1245
XY=    -8.5751   YY=    13.8439   ZY=   -25.2563
XZ=   -32.8465   YZ=   -23.8693   ZZ=   162.9299
Eigenvalues:   -55.4985    12.8492   172.2267
  15  C    Isotropic =    75.2847   Anisotropy =   116.4186
XX=    68.2490   YX=   -22.0712   ZX=   -17.9571
XY=   -26.9987   YY=    13.1969   ZY=   -25.6570
XZ=   -26.5979   YZ=   -24.5746   ZZ=   144.4084
Eigenvalues:    -2.9237    75.8808   152.8971
  16  C    Isotropic =   164.3659   Anisotropy =    40.9083
XX=   189.8660   YX=     5.2076   ZX=     3.1073
XY=     2.9732   YY=   158.2196   ZY=     2.3141
XZ=    11.4787   YZ=     3.9346   ZZ=   145.0121
Eigenvalues:   143.4393   158.0202   191.6381
  17  O    Isotropic =   216.0541   Anisotropy =    46.9955
XX=   179.4403   YX=     9.0114   ZX=    -5.8715
XY=    35.3530   YY=   233.1276   ZY=     6.2977
XZ=    -4.7201   YZ=    15.0274   ZZ=   235.5944
Eigenvalues:   170.3133   230.4646   247.3844
  18  C    Isotropic =    73.7127   Anisotropy =   123.7308
XX=    44.1686   YX=   -52.9359   ZX=   -34.3948
XY=   -46.5767   YY=    80.4098   ZY=   -64.8713
XZ=   -31.2695   YZ=   -67.9373   ZZ=    96.5596
Eigenvalues:   -27.3633    92.3014   156.1999
  19  C    Isotropic =   161.8180   Anisotropy =    35.4711
XX=   154.0903   YX=     4.4443   ZX=     6.3348
XY=     4.0336   YY=   173.1074   ZY=    15.6464
XZ=     1.4908   YZ=    18.7880   ZZ=   158.2564
Eigenvalues:   146.7945   153.1942   185.4654
  20  O    Isotropic =   280.4920   Anisotropy =    52.2017
XX=   280.3373   YX=    -1.7623   ZX=    -7.3264
XY=    -7.2187   YY=   269.6613   ZY=   -22.9066
XZ=   -42.5157   YZ=   -16.5129   ZZ=   291.4774
Eigenvalues:   247.5878   278.5951   315.2931
  21  H    Isotropic =    30.2412   Anisotropy =     8.5763
XX=    25.8708   YX=    -0.1670   ZX=    -0.4438
XY=     0.4349   YY=    33.8423   ZY=     3.0639
XZ=    -0.8250   YZ=     3.3964   ZZ=    31.0104
Eigenvalues:    25.7495    29.0154    35.9587
  22  H    Isotropic =    29.6548   Anisotropy =     6.1880
XX=    32.8498   YX=    -1.1008   ZX=    -2.0834
```

```
XY=    -1.2096   YY=    29.7672   ZY=    -0.1707
XZ=    -2.4410   YZ=    -0.9830   ZZ=    26.3475
Eigenvalues:    25.4473    29.7371    33.7801
  23  H    Isotropic =    29.9823   Anisotropy =     5.4257
XX=    32.2558   YX=    -0.3629   ZX=     2.8346
XY=    -0.7865   YY=    26.4847   ZY=    -0.4417
XZ=     0.7208   YZ=     0.9002   ZZ=    31.2064
Eigenvalues:    26.3903    29.9571    33.5994
  24  H    Isotropic =    29.9863   Anisotropy =     9.8604
XX=    27.8465   YX=     1.4643   ZX=    -2.6229
XY=     0.9431   YY=    27.1655   ZY=    -1.7971
XZ=    -3.9921   YZ=    -0.9214   ZZ=    34.9469
Eigenvalues:    26.0678    27.3313    36.5599
  25  H    Isotropic =    29.2603   Anisotropy =     7.1034
XX=    28.6848   YX=    -2.3226   ZX=     0.1015
XY=    -1.9959   YY=    32.4854   ZY=    -1.3035
XZ=    -0.7117   YZ=    -3.2629   ZZ=    26.6108
Eigenvalues:    25.4696    28.3155    33.9959
  26  H    Isotropic =    27.7458   Anisotropy =     5.6133
XX=    28.2098   YX=    -0.5692   ZX=    -0.3758
XY=     0.3149   YY=    28.5624   ZY=     2.9566
XZ=     1.2310   YZ=     4.6941   ZZ=    26.4651
Eigenvalues:    23.5102    28.2391    31.4879
  27  H    Isotropic =    28.1096   Anisotropy =     3.6536
XX=    28.5916   YX=     0.2774   ZX=    -2.4306
XY=     0.1367   YY=    25.9626   ZY=    -1.4500
XZ=     1.3609   YZ=    -1.8116   ZZ=    29.7746
Eigenvalues:    25.3602    28.4233    30.5454
  28  H    Isotropic =    30.6414   Anisotropy =     8.7694
XX=    27.1018   YX=    -0.0207   ZX=     0.1927
XY=     0.7161   YY=    36.0708   ZY=     2.3555
XZ=     0.3018   YZ=     1.1600   ZZ=    28.7515
Eigenvalues:    27.0644    28.3721    36.4876
  29  H    Isotropic =    30.6965   Anisotropy =     9.5824
XX=    27.9749   YX=     0.8506   ZX=    -1.8172
XY=     1.4649   YY=    31.6344   ZY=    -4.7289
XZ=    -2.1330   YZ=    -4.1815   ZZ=    32.4802
Eigenvalues:    27.0369    27.9678    37.0848
  30  H    Isotropic =    30.1366   Anisotropy =     8.1100
XX=    32.6891   YX=    -2.1374   ZX=     2.6104
XY=    -2.4568   YY=    31.4835   ZY=    -1.6541
XZ=     2.8565   YZ=    -1.6372   ZZ=    26.2374
Eigenvalues:    25.1313    29.7353    35.5433
  31  H    Isotropic =    25.7584   Anisotropy =     6.6138
XX=    28.8032   YX=     2.0262   ZX=     1.1947
XY=     1.7835   YY=    26.2452   ZY=     1.1723
XZ=     1.1279   YZ=     1.5116   ZZ=    22.2268
Eigenvalues:    21.7685    25.3391    30.1676
  32  H    Isotropic =    25.3046   Anisotropy =     8.1893
XX=    30.2995   YX=    -1.6465   ZX=     0.9874
XY=    -1.3935   YY=    24.4199   ZY=     0.1024
XZ=     0.9225   YZ=    -0.3142   ZZ=    21.1943
```

```
Eigenvalues:    21.0944    24.0552    30.7641
  33  H    Isotropic =    29.3623   Anisotropy =     8.8665
XX=    30.0687   YX=    -0.2491   ZX=     3.7221
XY=    -0.3049   YY=    26.3643   ZY=    -0.4822
XZ=     4.8978   YZ=    -0.3973   ZZ=    31.6538
Eigenvalues:    26.3072    26.5063    35.2733
  34  H    Isotropic =    29.7539   Anisotropy =     8.3516
XX=    33.6071   YX=    -3.0426   ZX=    -2.0035
XY=    -0.9304   YY=    29.4359   ZY=     2.6402
XZ=    -1.9964   YZ=     2.5773   ZZ=    26.2187
Eigenvalues:    24.6843    29.2558    35.3216
  35  H    Isotropic =    29.7266   Anisotropy =     7.8681
XX=    32.0838   YX=     3.7889   ZX=     0.0240
XY=     1.5285   YY=    32.3749   ZY=    -1.0907
XZ=    -0.4653   YZ=    -0.9779   ZZ=    24.7210
Eigenvalues:    24.5811    29.6267    34.9720
  36  H    Isotropic =    28.1331   Anisotropy =    14.9420
XX=    31.0258   YX=    -4.6189   ZX=     0.5584
XY=    -6.5161   YY=    33.5586   ZY=     1.6487
XZ=     0.1681   YZ=     2.2415   ZZ=    19.8148
Eigenvalues:    19.4121    26.8926    38.0944
  37  H    Isotropic =    26.5765   Anisotropy =     6.2212
XX=    28.5161   YX=     0.3665   ZX=    -1.8902
XY=    -1.2621   YY=    25.3930   ZY=     0.4657
XZ=    -4.5845   YZ=     0.0329   ZZ=    25.8206
Eigenvalues:    23.6606    25.3450    30.7240
  38  H    Isotropic =    26.4977   Anisotropy =     8.3326
XX=    30.1222   YX=    -1.3843   ZX=    -5.0359
XY=     1.1411   YY=    24.3127   ZY=    -0.2742
XZ=    -2.3135   YZ=    -0.1530   ZZ=    25.0581
Eigenvalues:    23.0787    24.3616    32.0527
  39  H    Isotropic =    28.9547   Anisotropy =     4.3142
XX=    26.8978   YX=     2.5348   ZX=     1.3495
XY=     2.2561   YY=    28.4014   ZY=    -0.1793
XZ=     0.6160   YZ=     0.0225   ZZ=    31.5648
Eigenvalues:    25.0305    30.0028    31.8308
  40  H    Isotropic =    29.8120   Anisotropy =     7.0376
XX=    30.7046   YX=    -0.5608   ZX=     0.5851
XY=    -2.0030   YY=    33.8561   ZY=     1.7524
XZ=    -0.4743   YZ=     1.1627   ZZ=    24.8752
Eigenvalues:    24.6335    30.2987    34.5037
  41  H    Isotropic =    29.7847   Anisotropy =     8.6866
XX=    32.2600   YX=     3.1062   ZX=    -0.9966
XY=     4.9316   YY=    30.6020   ZY=     1.5140
XZ=     0.1660   YZ=     1.4183   ZZ=    26.4920
Eigenvalues:    25.4265    28.3519    35.5757
  42  H    Isotropic =    29.8650   Anisotropy =    18.9450
XX=    32.0632   YX=     4.4656   ZX=    -5.8000
XY=     4.8794   YY=    25.0900   ZY=    -7.1153
XZ=    -5.7176   YZ=    -8.2449   ZZ=    32.4418
Eigenvalues:    20.1620    26.9379    42.4950
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 69.53 | 83.01 | 97.27 | 115.40 | 137.70 | 169.97 |
| intensities | 0.33 | 0.98 | 0.50 | 0.53 | 3.88 | 0.81 |
| reduc. mass | 1.82 | 0.93 | 1.11 | 0.93 | 2.86 | 1.14 |
| force const | 0.01 | 0.00 | 0.01 | 0.01 | 0.03 | 0.02 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 213.52 | 218.98 | 229.45 | 254.31 | 258.79 | 271.39 |
| intensities | 0.95 | 1.33 | 3.96 | 3.79 | 3.90 | 1.33 |
| reduc. mass | 0.74 | 0.69 | 0.40 | 0.71 | 1.51 | 1.89 |
| force const | 0.02 | 0.02 | 0.01 | 0.03 | 0.06 | 0.08 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 292.76 | 305.03 | 321.92 | 334.26 | 339.67 | 363.29 |
| intensities | 1.55 | 0.07 | 0.28 | 1.29 | 3.17 | 3.58 |
| reduc. mass | 0.28 | 0.78 | 0.67 | 0.27 | 0.72 | 0.60 |
| force const | 0.01 | 0.04 | 0.04 | 0.02 | 0.05 | 0.05 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|
| frequencies | 383.37 | 394.52 | 447.17 | 447.66 | 489.19 | 502.94 |
| intensities | 2.94 | 4.31 | 12.76 | 4.58 | 2.01 | 23.83 |
| reduc. mass | 0.73 | 0.59 | 0.72 | 0.86 | 0.93 | 0.62 |
| force const | 0.06 | 0.05 | 0.09 | 0.10 | 0.13 | 0.09 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 520.60 | 523.43 | 557.86 | 571.17 | 592.82 | 603.74 |
| intensities | 9.49 | 17.56 | 31.04 | 50.87 | 11.55 | 17.97 |
| reduc. mass | 1.33 | 0.77 | 0.38 | 0.40 | 0.81 | 1.62 |
| force const | 0.21 | 0.12 | 0.07 | 0.08 | 0.17 | 0.35 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 632.38 | 653.61 | 675.38 | 703.14 | 724.90 | 732.45 |
| intensities | 29.51 | 5.65 | 25.78 | 0.98 | 1.60 | 3.86 |
| reduc. mass | 0.50 | 0.75 | 0.84 | 1.35 | 0.32 | 0.45 |
| force const | 0.12 | 0.19 | 0.23 | 0.39 | 0.10 | 0.14 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 745.82 | 801.49 | 824.27 | 845.19 | 864.68 | 891.06 |
| intensities | 6.96 | 3.82 | 4.57 | 1.48 | 36.27 | 6.00 |
| reduc. mass | 1.11 | 0.79 | 0.92 | 3.04 | 0.54 | 0.89 |
| force const | 0.36 | 0.30 | 0.37 | 1.28 | 0.24 | 0.42 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|

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| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 904.46 | 931.04 | 951.16 | 993.91 | 1009.66 | 1010.81 |
| intensities | 12.49 | 0.74 | 10.70 | 1.51 | 20.35 | 17.74 |
| reduc. mass | 0.70 | 1.45 | 0.33 | 0.37 | 0.28 | 0.31 |
| force const | 0.34 | 0.74 | 0.18 | 0.22 | 0.17 | 0.18 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|

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| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 1029.37 | 1039.46 | 1049.96 | 1066.99 | 1088.19 | 1097.42 |
| intensities | 29.41 | 3.60 | 13.42 | 67.85 | 92.94 | 20.54 |
| reduc. mass | 0.31 | 0.32 | 0.27 | 0.43 | 0.41 | 0.32 |
| force const | 0.19 | 0.20 | 0.17 | 0.29 | 0.28 | 0.22 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|

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| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 1103.16 | 1114.16 | 1143.38 | 1179.82 | 1184.30 | 1217.36 |
| intensities | 31.06 | 20.64 | 11.80 | 31.45 | 6.96 | 75.43 |
| reduc. mass | 0.57 | 0.37 | 0.41 | 0.90 | 0.44 | 0.37 |
| force const | 0.41 | 0.27 | 0.31 | 0.74 | 0.36 | 0.32 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|

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| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 1222.27 | 1236.13 | 1248.46 | 1263.08 | 1317.05 | 1335.68 |
| intensities | 38.86 | 9.05 | 82.38 | 16.68 | 10.27 | 57.41 |
| reduc. mass | 0.26 | 0.31 | 0.76 | 0.26 | 1.88 | 0.94 |
| force const | 0.23 | 0.28 | 0.70 | 0.24 | 1.92 | 0.98 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|

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|---|---|---|---|---|---|---|
| frequencies | 1336.74 | 1372.34 | 1401.80 | 1431.89 | 1465.26 | 1483.60 |
| intensities | 99.10 | 33.83 | 78.67 | 687.14 | 64.52 | 40.03 |
| reduc. mass | 0.68 | 0.52 | 0.49 | 0.64 | 0.51 | 0.68 |
| force const | 0.71 | 0.57 | 0.56 | 0.77 | 0.64 | 0.89 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1484.73 | 1509.02 | 1511.88 | 1524.06 | 1526.11 | 1553.76 |
| intensities | 60.17 | 5.26 | 99.10 | 86.38 | 10.81 | 16.14 |
| reduc. mass | 0.53 | 0.69 | 1.32 | 1.41 | 0.66 | 0.59 |
| force const | 0.69 | 0.92 | 1.78 | 1.93 | 0.90 | 0.84 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1562.09 | 1572.59 | 1577.98 | 1619.40 | 1626.93 | 1641.25 |
| intensities | 19.74 | 28.10 | 22.14 | 89.11 | 2.17 | 1.21 |
| reduc. mass | 0.87 | 0.60 | 0.78 | 0.44 | 0.88 | 0.60 |
| force const | 1.25 | 0.88 | 1.14 | 0.68 | 1.37 | 0.96 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1650.59 | 1655.83 | 1658.98 | 1660.17 | 1662.73 | 1664.74 |
| intensities | 57.32 | 27.08 | 49.42 | 27.72 | 1.49 | 17.15 |
| reduc. mass | 0.17 | 0.45 | 0.15 | 0.30 | 0.16 | 0.29 |
| force const | 0.28 | 0.72 | 0.24 | 0.48 | 0.26 | 0.47 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1671.57 | 1678.63 | 1679.46 | 1682.20 | 1705.62 | 1794.20 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 31.53 | 1.99 | 5.11 | 56.45 | 41.76 | 1210.99 |
| reduc. mass | 0.19 | 0.34 | 0.38 | 1.10 | 1.05 | 1.41 |
| force const | 0.32 | 0.57 | 0.63 | 1.83 | 1.80 | 2.68 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1835.81 | 1891.22 | 3022.79 | 3026.82 | 3027.96 | 3058.55 |
| intensities | 290.89 | 22.72 | 316.54 | 462.27 | 711.10 | 284.51 |
| reduc. mass | 1.30 | 0.84 | 0.32 | 0.29 | 0.30 | 0.47 |
| force const | 2.59 | 1.78 | 1.74 | 1.58 | 1.60 | 2.58 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3067.35 | 3070.85 | 3087.69 | 3100.90 | 3110.41 | 3126.02 |
| intensities | 398.25 | 157.63 | 362.09 | 481.43 | 223.38 | 352.47 |
| reduc. mass | 0.35 | 0.34 | 0.92 | 0.47 | 0.89 | 0.34 |
| force const | 1.92 | 1.87 | 5.18 | 2.64 | 5.06 | 1.96 |

| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3129.67 | 3131.87 | 3136.03 | 3136.66 | 3144.42 | 3146.72 |
| intensities | 280.33 | 710.47 | 179.53 | 245.91 | 358.08 | 637.13 |
| reduc. mass | 0.29 | 0.21 | 0.26 | 0.77 | 0.53 | 0.49 |
| force const | 1.65 | 1.19 | 1.49 | 4.48 | 3.11 | 2.83 |

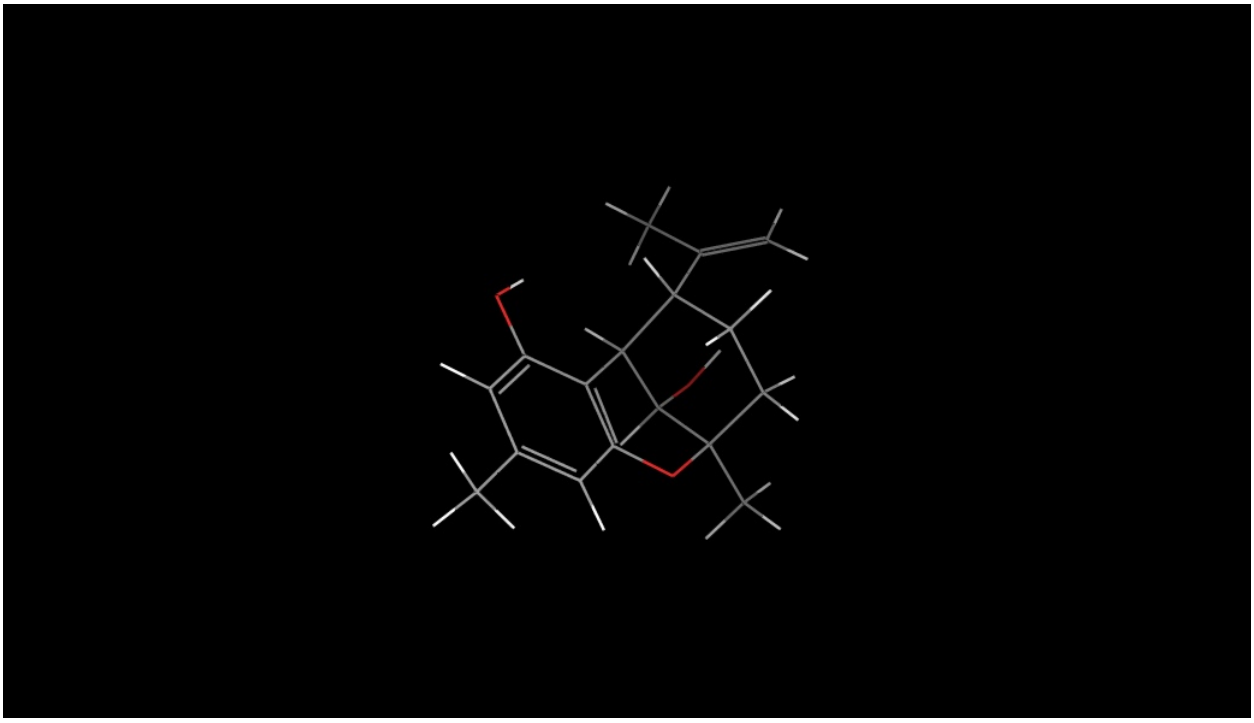
| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3147.56 | 3153.16 | 3154.78 | 3205.98 | 3835.99 | 3858.15 |
| intensities | 316.15 | 425.98 | 244.63 | 329.63 | 30.62 | 30.22 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.44 | 0.55 | 0.85 | 0.56 | 0.95 | 0.95 |
| force const | 2.58 | 3.20 | 5.01 | 3.40 | 8.21 | 8.31 |

Number of imaginary frequencies: 0

Conformation 2

Boltzmann Population = 2.7% (relative energy = 1.72 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.985612 hartrees

Total enthalpy, Htot (Utot + pV): -885.984668 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.045277 hartrees

Geometry Optimization:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.446800 | -1.908400 | 4.737200 |
| 2 | 6 | 0 | -1.088400 | -1.818400 | 3.247700 |
| 3 | 6 | 0 | -2.273300 | -1.386200 | 2.369700 |
| 4 | 6 | 0 | -2.893900 | -0.086800 | 2.968200 |
| 5 | 6 | 0 | -3.361500 | -0.295600 | 4.413800 |

| | | | | | |
|---|---|---|---|---|---|
| 6 | 6 | 0 | -2.134300 | -0.642800 | 5.272700 |
| 7 | 6 | 0 | -2.515300 | -0.801500 | 6.734400 |
| 8 | 6 | 0 | -3.310200 | -2.466700 | 2.093000 |
| 9 | 6 | 0 | -1.879100 | 1.029700 | 2.983700 |
| 10 | 6 | 0 | -1.097600 | 1.234800 | 4.124900 |
| 11 | 8 | 0 | -1.205900 | 0.456600 | 5.239700 |
| 12 | 6 | 0 | -1.650300 | 1.861700 | 1.880200 |
| 13 | 6 | 0 | -0.704000 | 2.879100 | 1.923500 |
| 14 | 6 | 0 | 0.048700 | 3.081900 | 3.080100 |
| 15 | 6 | 0 | -0.146800 | 2.252200 | 4.180100 |
| 16 | 6 | 0 | 1.049400 | 4.207700 | 3.142600 |
| 17 | 8 | 0 | -2.337500 | 1.705500 | 0.712700 |
| 18 | 6 | 0 | -3.179700 | -3.739300 | 2.480600 |
| 19 | 6 | 0 | -4.523700 | -2.026000 | 1.311300 |
| 20 | 8 | 0 | -4.392800 | -1.248300 | 4.543000 |
| 21 | 1 | 0 | -0.543300 | -2.079100 | 5.331100 |
| 22 | 1 | 0 | -2.111900 | -2.760000 | 4.926500 |
| 23 | 1 | 0 | -0.286900 | -1.084500 | 3.122800 |
| 24 | 1 | 0 | -0.685200 | -2.771800 | 2.894200 |
| 25 | 1 | 0 | -1.873500 | -1.105000 | 1.382300 |
| 26 | 1 | 0 | -3.775900 | 0.213100 | 2.386900 |
| 27 | 1 | 0 | -3.778500 | 0.646700 | 4.787700 |
| 28 | 1 | 0 | -1.627900 | -1.030700 | 7.330100 |
| 29 | 1 | 0 | -2.953100 | 0.128400 | 7.105800 |
| 30 | 1 | 0 | -3.247400 | -1.602800 | 6.846600 |
| 31 | 1 | 0 | -0.567300 | 3.499400 | 1.044100 |
| 32 | 1 | 0 | 0.431100 | 2.370900 | 5.090300 |
| 33 | 1 | 0 | 1.539600 | 4.353600 | 2.177000 |
| 34 | 1 | 0 | 0.555700 | 5.148300 | 3.407600 |
| 35 | 1 | 0 | 1.817800 | 4.012200 | 3.893800 |
| 36 | 1 | 0 | -2.981300 | 0.994800 | 0.806000 |
| 37 | 1 | 0 | -3.931500 | -4.477500 | 2.218800 |
| 38 | 1 | 0 | -2.328500 | -4.095700 | 3.050200 |
| 39 | 1 | 0 | -4.238000 | -1.392200 | 0.463000 |
| 40 | 1 | 0 | -5.075200 | -2.883900 | 0.922500 |
| 41 | 1 | 0 | -5.199100 | -1.445400 | 1.948200 |
| 42 | 1 | 0 | -4.094600 | -2.089900 | 4.171100 |

---

SCF GIAO Magnetic shielding tensor (ppm):

1 C Isotropic = 155.5305 Anisotropy = 29.9785

XX= 146.8676 YX= 5.1109 ZX= -7.4282

XY= 3.4891 YY= 156.3508 ZY= -8.0405

XZ= -13.4703 YZ= -13.6667 ZZ= 163.3730

Eigenvalues: 141.7272 149.3481 175.5161

2 C Isotropic = 165.2597 Anisotropy = 13.9946

XX= 156.7696 YX= -0.6375 ZX= -2.1744

XY= -1.1736 YY= 174.2994 ZY= 2.5099

XZ= 0.2214 YZ= 0.4879 ZZ= 164.7100

```
Eigenvalues:   156.6216   164.5680   174.5894
   3  C    Isotropic =   140.4787   Anisotropy =    21.7329
XX=   152.1590   YX=     9.2942   ZX=    14.2968
XY=     3.3618   YY=   137.9401   ZY=    -2.1290
XZ=    -5.4026   YZ=    -4.3592   ZZ=   131.3370
Eigenvalues:   128.1229   138.3458   154.9673
   4  C    Isotropic =   149.4323   Anisotropy =    21.7105
XX=   148.5175   YX=     2.6245   ZX=    -1.6809
XY=    -2.3059   YY=   137.3318   ZY=    -6.9847
XZ=     0.8079   YZ=    -5.4036   ZZ=   162.4476
Eigenvalues:   135.8870   148.5039   163.9060
   5  C    Isotropic =   110.9054   Anisotropy =    45.7256
XX=   140.7998   YX=     8.5643   ZX=     5.2439
XY=     0.9597   YY=   102.4583   ZY=    -3.8160
XZ=    -5.6489   YZ=    -2.6427   ZZ=    89.4583
Eigenvalues:    88.6846   102.6426   141.3892
   6  C    Isotropic =   108.8904   Anisotropy =    62.2236
XX=   146.9214   YX=    -0.7198   ZX=    11.8874
XY=     8.6614   YY=    86.3237   ZY=    -5.3622
XZ=    15.7580   YZ=    -7.0062   ZZ=    93.4262
Eigenvalues:    80.9476    95.3508   150.3728
   7  C    Isotropic =   160.3676   Anisotropy =    42.0159
XX=   147.8738   YX=    -8.2562   ZX=     0.1746
XY=    -8.0032   YY=   177.4291   ZY=   -19.2760
XZ=    -0.3825   YZ=   -15.6105   ZZ=   155.8000
Eigenvalues:   142.3681   150.3565   188.3782
   8  C    Isotropic =    27.2800   Anisotropy =   194.2849
XX=   -16.2912   YX=   -50.2445   ZX=   -27.3455
XY=   -49.2970   YY=    40.8141   ZY=  -111.6543
XZ=   -31.0513   YZ=  -101.2468   ZZ=    57.3172
Eigenvalues:   -97.2404    22.2772   156.8033
   9  C    Isotropic =    77.3427   Anisotropy =   119.5724
XX=    31.7846   YX=    -1.6869   ZX=   -23.9911
XY=     0.3863   YY=    49.6782   ZY=   -17.9718
XZ=   -21.6221   YZ=   -13.9681   ZZ=   150.5655
Eigenvalues:    26.9508    48.0198   157.0577
  10  C    Isotropic =    25.8125   Anisotropy =   136.4685
XX=    -7.3113   YX=    38.9204   ZX=   -13.8034
XY=    44.7164   YY=   -25.7396   ZY=   -18.2745
XZ=   -14.9860   YZ=   -20.8138   ZZ=   110.4885
Eigenvalues:   -59.5831    20.2292   116.7915
  11  O    Isotropic =   173.6479   Anisotropy =    60.5271
XX=   128.4494   YX=    -1.7481   ZX=   -16.5906
XY=   -30.7145   YY=   187.1885   ZY=    -2.2099
XZ=   -10.6028   YZ=   -27.8513   ZZ=   205.3059
Eigenvalues:   120.8026   186.1418   213.9993
  12  C    Isotropic =    28.6726   Anisotropy =   131.4222
XX=    17.9883   YX=   -25.6940   ZX=   -20.2985
XY=   -22.3630   YY=   -42.8671   ZY=   -23.1894
XZ=   -16.7406   YZ=   -20.0102   ZZ=   110.8968
Eigenvalues:   -55.4594    25.1899   116.2875
  13  C    Isotropic =    77.1670   Anisotropy =   118.9191
```

```
XX=    49.4683   YX=    33.5581   ZX=   -12.4066
XY=    39.3596   YY=    27.7190   ZY=   -11.0355
XZ=    -4.5790   YZ=    -9.2237   ZZ=   154.3137
Eigenvalues:     0.4864    74.5683   156.4464
  14  C    Isotropic =    41.6004   Anisotropy =   196.9421
XX=   -50.4284   YX=    -6.0477   ZX=   -34.6851
XY=    -6.3256   YY=    11.1603   ZY=   -23.7139
XZ=   -35.8373   YZ=   -24.1277   ZZ=   164.0693
Eigenvalues:   -57.5488     9.4549   172.8951
  15  C    Isotropic =    76.2531   Anisotropy =   113.8037
XX=    68.9690   YX=   -21.0060   ZX=   -15.8469
XY=   -27.6768   YY=    13.4338   ZY=   -25.4429
XZ=   -10.8088   YZ=   -26.0638   ZZ=   146.3566
Eigenvalues:    -1.3449    77.9820   152.1222
  16  C    Isotropic =   164.0599   Anisotropy =    40.9816
XX=   189.1246   YX=     4.8683   ZX=    12.6046
XY=     4.1064   YY=   158.1322   ZY=     3.4778
XZ=     4.0811   YZ=     2.3134   ZZ=   144.9230
Eigenvalues:   143.1130   157.6858   191.3810
  17  O    Isotropic =   222.1072   Anisotropy =    82.0383
XX=   173.2220   YX=    10.5439   ZX=   -14.1387
XY=    23.8308   YY=   219.0167   ZY=    -1.7879
XZ=    -0.7264   YZ=    26.1567   ZZ=   274.0828
Eigenvalues:   166.3698   223.1524   276.7994
  18  C    Isotropic =    71.8695   Anisotropy =   126.0801
XX=    38.3570   YX=   -51.6902   ZX=   -36.0831
XY=   -45.0784   YY=    83.7645   ZY=   -64.9757
XZ=   -33.3422   YZ=   -68.0287   ZZ=    93.4870
Eigenvalues:   -29.6195    89.3052   155.9229
  19  C    Isotropic =   161.2275   Anisotropy =    35.2401
XX=   153.9886   YX=     4.4399   ZX=     6.9134
XY=     3.9202   YY=   171.9697   ZY=    15.9794
XZ=     2.6612   YZ=    18.4845   ZZ=   157.7241
Eigenvalues:   145.8185   153.1431   184.7209
  20  O    Isotropic =   278.9242   Anisotropy =    52.2820
XX=   278.2628   YX=    -2.8547   ZX=    -8.1891
XY=    -8.5020   YY=   267.8862   ZY=   -21.3791
XZ=   -43.9221   YZ=   -13.9148   ZZ=   290.6237
Eigenvalues:   245.9728   277.0209   313.7789
  21  H    Isotropic =    30.2115   Anisotropy =     8.6174
XX=    25.8951   YX=    -0.0997   ZX=    -0.3807
XY=     0.5317   YY=    33.7651   ZY=     3.1286
XZ=    -0.7707   YZ=     3.4756   ZZ=    30.9743
Eigenvalues:    25.7740    28.9041    35.9564
  22  H    Isotropic =    29.7060   Anisotropy =     6.2457
XX=    32.9161   YX=    -1.0904   ZX=    -2.1075
XY=    -1.1698   YY=    29.8880   ZY=    -0.1352
XZ=    -2.5479   YZ=    -0.9301   ZZ=    26.3138
Eigenvalues:    25.4108    29.8374    33.8698
  23  H    Isotropic =    29.9314   Anisotropy =     5.3894
XX=    32.3595   YX=    -0.4895   ZX=     2.7294
XY=    -0.8002   YY=    26.3437   ZY=    -0.4303
```

```
XZ=     0.5928   YZ=     0.9420   ZZ=    31.0912
Eigenvalues:    26.2337    30.0362    33.5244
  24  H    Isotropic =    29.9858   Anisotropy =     9.9499
XX=    27.8329   YX=     1.4551   ZX=    -2.6126
XY=     0.9548   YY=    27.0940   ZY=    -1.7977
XZ=    -3.9906   YZ=    -0.9054   ZZ=    35.0306
Eigenvalues:    26.0344    27.3039    36.6190
  25  H    Isotropic =    29.5160   Anisotropy =     6.8928
XX=    28.7879   YX=    -2.1662   ZX=     0.0538
XY=    -1.8799   YY=    32.6520   ZY=    -1.3867
XZ=    -0.9207   YZ=    -3.3291   ZZ=    27.1080
Eigenvalues:    25.7744    28.6623    34.1112
  26  H    Isotropic =    28.3560   Anisotropy =     5.1284
XX=    28.6567   YX=    -0.2816   ZX=    -0.3225
XY=     0.3161   YY=    28.8165   ZY=     2.5658
XZ=     1.5615   YZ=     4.3561   ZZ=    27.5949
Eigenvalues:    24.6375    28.6556    31.7749
  27  H    Isotropic =    28.0487   Anisotropy =     3.6300
XX=    28.5667   YX=     0.2814   ZX=    -2.4173
XY=     0.1154   YY=    25.9272   ZY=    -1.5430
XZ=     1.4442   YZ=    -1.8932   ZZ=    29.6522
Eigenvalues:    25.2558    28.4216    30.4687
  28  H    Isotropic =    30.6092   Anisotropy =     8.8206
XX=    27.0945   YX=     0.0187   ZX=     0.2548
XY=     0.7774   YY=    36.0561   ZY=     2.3843
XZ=     0.3481   YZ=     1.1963   ZZ=    28.6770
Eigenvalues:    27.0384    28.2996    36.4896
  29  H    Isotropic =    30.6740   Anisotropy =     9.6152
XX=    27.9214   YX=     0.8448   ZX=    -1.8004
XY=     1.4880   YY=    31.6395   ZY=    -4.7552
XZ=    -2.1155   YZ=    -4.1842   ZZ=    32.4610
Eigenvalues:    27.0146    27.9231    37.0841
  30  H    Isotropic =    30.1952   Anisotropy =     8.1514
XX=    32.7443   YX=    -2.1857   ZX=     2.5531
XY=    -2.5316   YY=    31.5764   ZY=    -1.6529
XZ=     2.8029   YZ=    -1.6148   ZZ=    26.2649
Eigenvalues:    25.2015    29.7545    35.6294
  31  H    Isotropic =    25.2917   Anisotropy =     6.7713
XX=    28.4881   YX=     2.1622   ZX=     1.3539
XY=     1.7182   YY=    25.9498   ZY=     0.9567
XZ=     1.2239   YZ=     0.5792   ZZ=    21.4372
Eigenvalues:    21.1676    24.9015    29.8059
  32  H    Isotropic =    25.3336   Anisotropy =     8.2809
XX=    30.4516   YX=    -1.7046   ZX=     1.0469
XY=    -1.2444   YY=    24.2169   ZY=     0.2936
XZ=     0.8226   YZ=     0.5227   ZZ=    21.3323
Eigenvalues:    21.1303    24.0164    30.8542
  33  H    Isotropic =    29.6172   Anisotropy =     8.2022
XX=    31.7046   YX=    -2.9097   ZX=     3.0877
XY=    -1.0716   YY=    30.5081   ZY=    -1.8503
XZ=     3.7126   YZ=    -2.4197   ZZ=    26.6388
Eigenvalues:    24.7226    29.0437    35.0853
```

```
  34  H    Isotropic =    29.3129   Anisotropy =     9.0885
XX=    32.6866   YX=     0.6978   ZX=    -3.4890
XY=     1.1183   YY=    26.4096   ZY=    -0.1810
XZ=    -4.6933   YZ=    -0.2548   ZZ=    28.8426
Eigenvalues:    25.9795    26.5874    35.3719
  35  H    Isotropic =    29.7593   Anisotropy =     7.6857
XX=    31.2600   YX=     2.6225   ZX=     2.5558
XY=     0.3776   YY=    31.2168   ZY=     3.1860
XZ=     2.3093   YZ=     3.6627   ZZ=    26.8009
Eigenvalues:    24.5958    29.7989    34.8831
  36  H    Isotropic =    27.6509   Anisotropy =    13.5470
XX=    36.2006   YX=    -1.5471   ZX=     2.6625
XY=     0.2543   YY=    28.9442   ZY=     2.8215
XZ=     3.2482   YZ=     0.5972   ZZ=    17.8079
Eigenvalues:    17.0750    29.1955    36.6823
  37  H    Isotropic =    26.5051   Anisotropy =     6.2356
XX=    28.3347   YX=     0.2718   ZX=    -1.9332
XY=    -1.2206   YY=    25.3731   ZY=     0.5142
XZ=    -4.6583   YZ=     0.1179   ZZ=    25.8076
Eigenvalues:    23.5414    25.3118    30.6622
  38  H    Isotropic =    26.4307   Anisotropy =     8.4046
XX=    30.0291   YX=    -1.3581   ZX=    -5.0847
XY=     1.0764   YY=    24.2428   ZY=    -0.2010
XZ=    -2.4139   YZ=    -0.1194   ZZ=    25.0202
Eigenvalues:    22.9816    24.2767    32.0337
  39  H    Isotropic =    30.1196   Anisotropy =     7.3480
XX=    30.4499   YX=    -0.3660   ZX=     0.6405
XY=    -1.7904   YY=    34.5667   ZY=     1.6894
XZ=    -0.4099   YZ=     1.1263   ZZ=    25.3421
Eigenvalues:    25.1177    30.2228    35.0182
  40  H    Isotropic =    29.6568   Anisotropy =     8.6586
XX=    32.5318   YX=     3.0175   ZX=    -0.7909
XY=     4.7356   YY=    30.0456   ZY=     1.6403
XZ=     0.4146   YZ=     1.5298   ZZ=    26.3929
Eigenvalues:    25.3146    28.2264    35.4292
  41  H    Isotropic =    28.8261   Anisotropy =     4.0918
XX=    26.8385   YX=     2.7002   ZX=     1.2837
XY=     2.3677   YY=    28.3086   ZY=    -0.2048
XZ=     0.4654   YZ=    -0.0592   ZZ=    31.3311
Eigenvalues:    24.8413    30.0830    31.5539
  42  H    Isotropic =    30.0051   Anisotropy =    17.9365
XX=    32.5099   YX=     3.9150   ZX=    -5.9510
XY=     4.3125   YY=    24.6393   ZY=    -6.0228
XZ=    -5.8989   YZ=    -7.1085   ZZ=    32.8662
Eigenvalues:    20.9405    27.1121    41.9628
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 70.87 | 85.53 | 96.84 | 127.11 | 138.18 | 171.42 |
| intensities | 0.33 | 1.25 | 0.14 | 2.30 | 3.66 | 1.16 |
| reduc. mass | 1.60 | 0.80 | 1.26 | 1.85 | 2.18 | 1.30 |
| force const | 0.00 | 0.00 | 0.01 | 0.02 | 0.02 | 0.02 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 214.48 | 221.57 | 245.28 | 254.39 | 262.27 | 282.36 |
| intensities | 0.25 | 0.55 | 5.75 | 2.03 | 2.54 | 6.18 |
| reduc. mass | 0.87 | 0.83 | 1.51 | 0.78 | 1.08 | 2.05 |
| force const | 0.02 | 0.02 | 0.05 | 0.03 | 0.04 | 0.10 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 294.85 | 311.12 | 321.08 | 332.46 | 337.34 | 355.39 |
| intensities | 1.29 | 0.96 | 2.24 | 1.49 | 2.72 | 1.07 |
| reduc. mass | 0.22 | 0.23 | 0.67 | 0.25 | 0.62 | 0.67 |
| force const | 0.01 | 0.01 | 0.04 | 0.02 | 0.04 | 0.05 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 379.30 | 382.64 | 413.55 | 443.43 | 463.99 | 491.08 |
| intensities | 5.97 | 9.38 | 13.19 | 1.62 | 26.64 | 6.81 |
| reduc. mass | 0.46 | 0.58 | 0.35 | 0.73 | 0.35 | 1.28 |
| force const | 0.04 | 0.05 | 0.04 | 0.09 | 0.04 | 0.18 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 509.52 | 523.55 | 526.67 | 563.12 | 588.64 | 598.75 |
| intensities | 15.34 | 7.35 | 16.49 | 9.70 | 7.68 | 16.45 |
| reduc. mass | 0.70 | 2.20 | 0.81 | 0.68 | 0.50 | 0.87 |
| force const | 0.11 | 0.35 | 0.13 | 0.13 | 0.10 | 0.18 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 620.79 | 660.33 | 686.39 | 699.99 | 727.84 | 739.49 |
| intensities | 34.81 | 20.60 | 36.20 | 2.14 | 5.53 | 1.96 |
| reduc. mass | 0.52 | 0.87 | 0.41 | 1.19 | 0.35 | 0.50 |
| force const | 0.12 | 0.22 | 0.11 | 0.34 | 0.11 | 0.16 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 753.96 | 800.36 | 822.69 | 828.24 | 863.38 | 891.32 |
| intensities | 0.74 | 3.67 | 4.96 | 2.26 | 28.10 | 2.31 |
| reduc. mass | 1.86 | 0.84 | 0.95 | 1.36 | 0.59 | 0.81 |
| force const | 0.62 | 0.32 | 0.38 | 0.55 | 0.26 | 0.38 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 904.20 | 931.86 | 952.84 | 993.89 | 1006.33 | 1012.89 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 13.74 | 1.53 | 14.04 | 0.64 | 4.11 | 24.57 |
| reduc. mass | 0.70 | 1.53 | 0.31 | 0.34 | 0.31 | 0.28 |
| force const | 0.34 | 0.78 | 0.16 | 0.20 | 0.18 | 0.17 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1026.93 | 1034.39 | 1044.74 | 1059.88 | 1081.96 | 1095.11 |
| intensities | 39.38 | 19.48 | 16.31 | 31.01 | 5.73 | 17.54 |
| reduc. mass | 0.28 | 0.28 | 0.29 | 0.28 | 0.40 | 0.57 |
| force const | 0.17 | 0.18 | 0.19 | 0.19 | 0.28 | 0.41 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1102.10 | 1114.67 | 1155.36 | 1168.95 | 1202.86 | 1207.57 |
| intensities | 10.84 | 54.71 | 8.06 | 10.92 | 10.67 | 282.63 |
| reduc. mass | 0.56 | 0.43 | 0.74 | 0.91 | 0.64 | 0.42 |
| force const | 0.40 | 0.32 | 0.59 | 0.73 | 0.55 | 0.36 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1220.53 | 1235.65 | 1257.79 | 1263.82 | 1317.91 | 1332.71 |
| intensities | 36.57 | 14.32 | 131.78 | 7.18 | 10.16 | 127.00 |
| reduc. mass | 0.29 | 0.34 | 0.91 | 0.28 | 1.65 | 0.55 |
| force const | 0.25 | 0.30 | 0.85 | 0.27 | 1.68 | 0.58 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1338.90 | 1370.54 | 1397.31 | 1417.01 | 1462.30 | 1480.67 |
| intensities | 40.13 | 24.41 | 35.06 | 682.63 | 32.09 | 23.83 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.58 | 0.45 | 0.49 | 0.89 | 0.69 | 0.55 |
| force const | 0.61 | 0.50 | 0.56 | 1.05 | 0.88 | 0.71 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1489.02 | 1504.32 | 1519.45 | 1523.34 | 1526.95 | 1554.15 |
| intensities | 100.61 | 3.01 | 214.63 | 13.55 | 71.85 | 8.79 |
| reduc. mass | 0.95 | 0.75 | 1.32 | 0.82 | 1.03 | 0.68 |
| force const | 1.24 | 1.00 | 1.79 | 1.12 | 1.41 | 0.97 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1558.30 | 1573.16 | 1582.94 | 1613.90 | 1628.98 | 1644.50 |
| intensities | 15.00 | 17.01 | 18.65 | 83.59 | 20.78 | 3.87 |
| reduc. mass | 0.85 | 0.66 | 0.74 | 0.36 | 0.73 | 0.54 |
| force const | 1.21 | 0.96 | 1.09 | 0.55 | 1.15 | 0.87 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1649.40 | 1658.37 | 1659.86 | 1660.97 | 1661.63 | 1664.11 |
| intensities | 102.11 | 29.66 | 30.85 | 18.40 | 11.18 | 18.80 |
| reduc. mass | 0.29 | 0.17 | 0.24 | 0.24 | 0.36 | 0.17 |
| force const | 0.46 | 0.28 | 0.39 | 0.38 | 0.59 | 0.28 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1672.83 | 1678.14 | 1679.14 | 1687.04 | 1707.20 | 1798.05 |
| intensities | 37.99 | 2.48 | 4.62 | 192.92 | 44.12 | 1267.01 |
| reduc. mass | 0.24 | 0.37 | 0.38 | 1.50 | 1.06 | 1.38 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 0.39 | 0.62 | 0.63 | 2.52 | 1.82 | 2.62 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1830.17 | 1892.12 | 3020.84 | 3027.26 | 3029.22 | 3058.96 |
| intensities | 361.28 | 20.79 | 338.42 | 510.39 | 634.34 | 263.06 |
| reduc. mass | 1.29 | 0.85 | 0.34 | 0.25 | 0.25 | 0.48 |
| force const | 2.55 | 1.80 | 1.80 | 1.36 | 1.37 | 2.63 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3059.40 | 3071.54 | 3082.97 | 3090.85 | 3103.12 | 3125.79 |
| intensities | 294.07 | 294.84 | 301.71 | 290.86 | 518.29 | 250.53 |
| reduc. mass | 0.83 | 0.43 | 0.84 | 0.87 | 0.48 | 0.20 |
| force const | 4.57 | 2.39 | 4.73 | 4.89 | 2.72 | 1.15 |

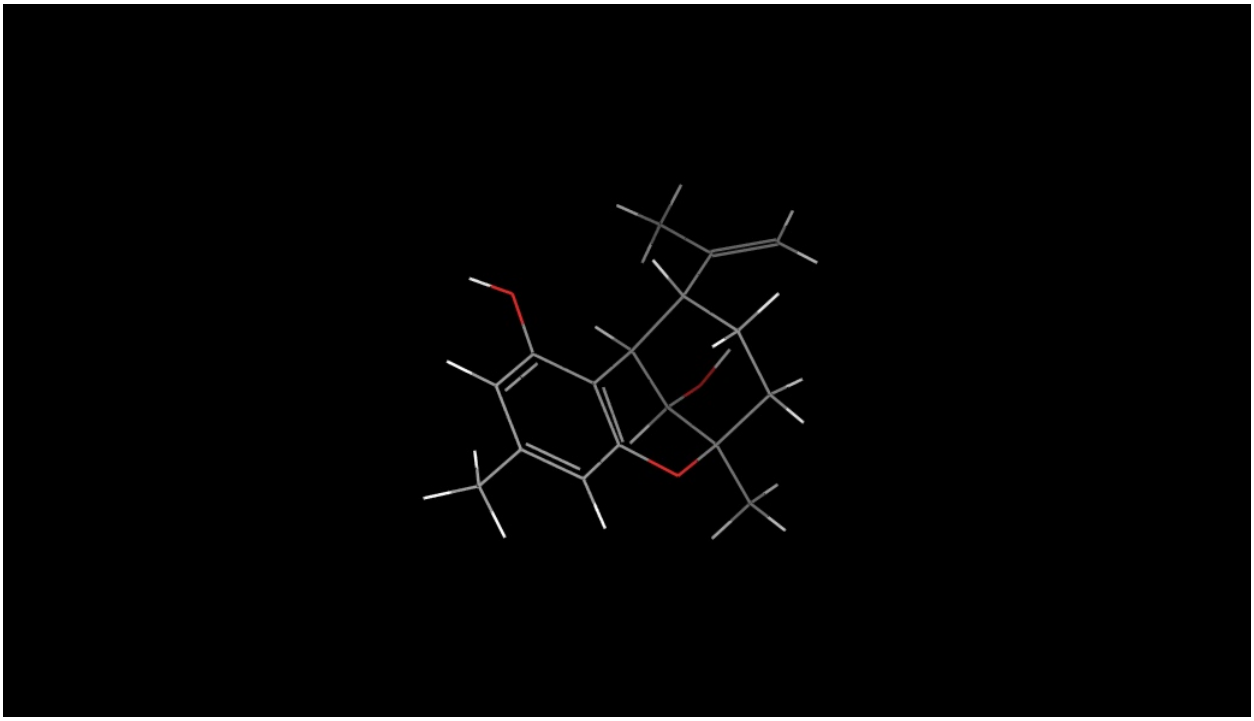
| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3127.21 | 3131.90 | 3136.40 | 3145.23 | 3146.25 | 3147.72 |
| intensities | 325.31 | 261.40 | 560.88 | 363.50 | 581.37 | 173.12 |
| reduc. mass | 0.26 | 0.18 | 0.31 | 0.53 | 0.58 | 0.46 |
| force const | 1.47 | 1.03 | 1.79 | 3.09 | 3.36 | 2.70 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3152.77 | 3154.54 | 3155.82 | 3205.37 | 3837.79 | 3857.40 |
| intensities | 414.10 | 536.92 | 123.04 | 328.97 | 23.28 | 13.04 |
| reduc. mass | 0.52 | 0.43 | 0.47 | 0.57 | 0.95 | 0.95 |
| force const | 3.07 | 2.53 | 2.75 | 3.43 | 8.22 | 8.31 |

Number of imaginary frequencies: 0

Conformation 3

Boltzmann Population = 49.3% (relative energy = 0.00 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.988429 hartrees

Total enthalpy, Htot (Utot + pV): -885.987485 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.048189 hartrees

Optimized geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.363700 | -1.965000 | 4.792800 |
| 2 | 6 | 0 | -1.015000 | -1.886700 | 3.300200 |
| 3 | 6 | 0 | -2.211000 | -1.492900 | 2.420000 |

| | | | | | |
|---|---|---|---|---|---|
| 4 | 6 | 0 | -2.878700 | -0.213600 | 3.006000 |
| 5 | 6 | 0 | -3.327800 | -0.418500 | 4.456200 |
| 6 | 6 | 0 | -2.083700 | -0.712100 | 5.313600 |
| 7 | 6 | 0 | -2.447200 | -0.855400 | 6.780900 |
| 8 | 6 | 0 | -3.215800 | -2.601200 | 2.141800 |
| 9 | 6 | 0 | -1.896200 | 0.926400 | 3.008200 |
| 10 | 6 | 0 | -1.112100 | 1.176100 | 4.132700 |
| 11 | 8 | 0 | -1.183600 | 0.414600 | 5.257600 |
| 12 | 6 | 0 | -1.714900 | 1.747600 | 1.890700 |
| 13 | 6 | 0 | -0.806900 | 2.798200 | 1.901100 |
| 14 | 6 | 0 | -0.041500 | 3.046800 | 3.046500 |
| 15 | 6 | 0 | -0.195000 | 2.232000 | 4.159200 |
| 16 | 6 | 0 | 0.944800 | 4.187300 | 3.053100 |
| 17 | 8 | 0 | -2.475200 | 1.445700 | 0.796600 |
| 18 | 6 | 0 | -3.064700 | -3.865800 | 2.549300 |
| 19 | 6 | 0 | -4.424300 | -2.190200 | 1.336500 |
| 20 | 8 | 0 | -4.319800 | -1.408900 | 4.614900 |
| 21 | 1 | 0 | -0.453700 | -2.105400 | 5.385200 |
| 22 | 1 | 0 | -2.008200 | -2.829000 | 4.996400 |
| 23 | 1 | 0 | -0.229900 | -1.136700 | 3.163300 |
| 24 | 1 | 0 | -0.590100 | -2.835700 | 2.959500 |
| 25 | 1 | 0 | -1.828600 | -1.195400 | 1.432400 |
| 26 | 1 | 0 | -3.740500 | 0.066800 | 2.394700 |
| 27 | 1 | 0 | -3.776300 | 0.512800 | 4.822800 |
| 28 | 1 | 0 | -1.550100 | -1.054600 | 7.373200 |
| 29 | 1 | 0 | -2.903200 | 0.070500 | 7.140700 |
| 30 | 1 | 0 | -3.160100 | -1.671000 | 6.910500 |
| 31 | 1 | 0 | -0.688400 | 3.424400 | 1.019200 |
| 32 | 1 | 0 | 0.388000 | 2.389000 | 5.060100 |
| 33 | 1 | 0 | 1.707300 | 4.049500 | 2.280300 |
| 34 | 1 | 0 | 0.443700 | 5.138900 | 2.851800 |
| 35 | 1 | 0 | 1.450200 | 4.267200 | 4.017500 |
| 36 | 1 | 0 | -2.287100 | 2.082700 | 0.098500 |
| 37 | 1 | 0 | -3.795400 | -4.624200 | 2.284600 |
| 38 | 1 | 0 | -2.214700 | -4.195900 | 3.136700 |
| 39 | 1 | 0 | -5.135900 | -1.651000 | 1.970700 |
| 40 | 1 | 0 | -4.139500 | -1.516100 | 0.521400 |
| 41 | 1 | 0 | -4.932300 | -3.059700 | 0.915100 |
| 42 | 1 | 0 | -4.017700 | -2.227000 | 4.196300 |

---

```
Calculating GIAO nuclear magnetic shielding tensors.
 SCF GIAO Magnetic shielding tensor (ppm):
      1  C    Isotropic =   155.1828   Anisotropy =    30.0317
   XX=   146.2775   YX=     4.9659   ZX=    -7.7531
   XY=     3.3801   YY=   156.3030   ZY=    -7.8666
   XZ=   -13.7499   YZ=   -13.5900   ZZ=   162.9678
   Eigenvalues:   140.9233   149.4211   175.2039
      2  C    Isotropic =   165.0725   Anisotropy =    13.9653
```

```
XX=   156.5747   YX=    -0.5833   ZX=    -2.5056
XY=    -1.2925   YY=   174.0822   ZY=     2.3912
XZ=     0.0700   YZ=     0.6078   ZZ=   164.5605
Eigenvalues:   156.3644   164.4703   174.3827
   3  C    Isotropic =   140.8539   Anisotropy =    21.2693
XX=   151.8619   YX=     9.8795   ZX=    13.1906
XY=     3.9895   YY=   138.8192   ZY=    -2.0079
XZ=    -5.9337   YZ=    -4.9155   ZZ=   131.8806
Eigenvalues:   128.7283   138.7999   155.0335
   4  C    Isotropic =   149.7840   Anisotropy =    19.7113
XX=   150.5472   YX=     2.2269   ZX=    -1.3480
XY=    -3.2846   YY=   137.7404   ZY=    -8.1019
XZ=     2.4347   YZ=    -5.4479   ZZ=   161.0643
Eigenvalues:   135.9060   150.5211   162.9249
   5  C    Isotropic =   111.2106   Anisotropy =    45.8554
XX=   141.2222   YX=     8.4354   ZX=     5.0017
XY=     0.8169   YY=   102.1342   ZY=    -3.4134
XZ=    -6.2783   YZ=    -2.5420   ZZ=    90.2754
Eigenvalues:    89.5658   102.2851   141.7809
   6  C    Isotropic =   107.9125   Anisotropy =    63.7005
XX=   146.8115   YX=    -0.8753   ZX=    12.2357
XY=     8.6073   YY=    84.6035   ZY=    -4.9031
XZ=    16.1831   YZ=    -6.8676   ZZ=    92.3224
Eigenvalues:    79.7040    93.6539   150.3795
   7  C    Isotropic =   160.3698   Anisotropy =    41.9490
XX=   147.7335   YX=    -8.3362   ZX=     0.2590
XY=    -8.0358   YY=   177.4243   ZY=   -19.1606
XZ=    -0.3588   YZ=   -15.4954   ZZ=   155.9516
Eigenvalues:   142.4211   150.3526   188.3358
   8  C    Isotropic =    25.1458   Anisotropy =   197.3051
XX=   -17.1061   YX=   -50.5760   ZX=   -23.8942
XY=   -49.5900   YY=    33.1125   ZY=  -113.8449
XZ=   -27.2396   YZ=  -102.9131   ZZ=    59.4312
Eigenvalues:   -99.3050    18.0600   156.6826
   9  C    Isotropic =    73.3015   Anisotropy =   127.8937
XX=    26.9624   YX=     1.2387   ZX=   -24.1023
XY=     3.2540   YY=    40.7167   ZY=   -20.0095
XZ=   -20.1853   YZ=   -14.3220   ZZ=   152.2254
Eigenvalues:    23.1322    38.2084   158.5640
  10  C    Isotropic =    24.6192   Anisotropy =   138.9214
XX=   -13.1401   YX=    37.6425   ZX=   -14.7057
XY=    45.6550   YY=   -23.7110   ZY=   -18.0571
XZ=   -15.7588   YZ=   -21.4315   ZZ=   110.7087
Eigenvalues:   -60.5455    17.1696   117.2335
  11  O    Isotropic =   170.1189   Anisotropy =    68.7492
XX=   122.7174   YX=    -2.4467   ZX=   -18.1844
XY=   -30.5263   YY=   181.1352   ZY=    -4.1280
XZ=   -12.6953   YZ=   -30.9853   ZZ=   206.5041
Eigenvalues:   114.2023   180.2027   215.9517
  12  C    Isotropic =    29.1512   Anisotropy =   130.0312
XX=    21.3768   YX=   -27.7333   ZX=   -19.4852
XY=   -17.6822   YY=   -44.2198   ZY=   -23.7280
```

```
XZ=   -15.5612   YZ=   -22.3405   ZZ=   110.2965
Eigenvalues:   -55.8026    27.4175   115.8387
  13  C    Isotropic =    80.6698   Anisotropy =   101.8142
XX=    60.5363   YX=    36.0094   ZX=    -9.4075
XY=    44.9230   YY=    35.7828   ZY=    -8.8923
XZ=    -8.7277   YZ=    -9.6704   ZZ=   145.6903
Eigenvalues:     5.8119    87.6515   148.5459
  14  C    Isotropic =    43.2550   Anisotropy =   193.2939
XX=   -47.2711   YX=    -9.0271   ZX=   -36.7550
XY=    -8.7210   YY=    14.0109   ZY=   -24.6821
XZ=   -34.4090   YZ=   -23.9761   ZZ=   163.0252
Eigenvalues:   -55.5290    13.1765   172.1176
  15  C    Isotropic =    74.7773   Anisotropy =   112.5149
XX=    68.8997   YX=   -23.2985   ZX=   -16.7766
XY=   -27.2275   YY=    12.6138   ZY=   -25.4847
XZ=   -18.6881   YZ=   -25.5101   ZZ=   142.8186
Eigenvalues:    -3.3125    77.8573   149.7873
  16  C    Isotropic =   164.4513   Anisotropy =    41.0520
XX=   188.9955   YX=     9.2530   ZX=     8.0502
XY=     3.5294   YY=   159.0099   ZY=     3.0057
XZ=     7.6785   YZ=     3.8547   ZZ=   145.3485
Eigenvalues:   143.6135   157.9210   191.8193
  17  O    Isotropic =   216.2578   Anisotropy =    46.4307
XX=   179.3834   YX=     8.8581   ZX=    -5.9592
XY=    35.0712   YY=   234.0019   ZY=     6.3508
XZ=    -3.7892   YZ=    13.5334   ZZ=   235.3880
Eigenvalues:   170.6691   230.8926   247.2116
  18  C    Isotropic =    73.7090   Anisotropy =   123.6402
XX=    44.1945   YX=   -52.7342   ZX=   -34.6229
XY=   -46.3082   YY=    80.5987   ZY=   -64.9030
XZ=   -31.6041   YZ=   -67.9677   ZZ=    96.3338
Eigenvalues:   -27.3551    92.3463   156.1358
  19  C    Isotropic =   161.8134   Anisotropy =    35.5185
XX=   154.0903   YX=     4.4268   ZX=     6.3255
XY=     4.0375   YY=   173.0459   ZY=    15.7023
XZ=     1.5569   YZ=    18.8454   ZZ=   158.3040
Eigenvalues:   146.7530   153.1948   185.4924
  20  O    Isotropic =   280.5432   Anisotropy =    52.2696
XX=   280.5954   YX=    -1.7424   ZX=    -7.4590
XY=    -7.1820   YY=   269.7994   ZY=   -22.9389
XZ=   -42.8004   YZ=   -16.3905   ZZ=   291.2350
Eigenvalues:   247.5546   278.6855   315.3897
  21  H    Isotropic =    30.2420   Anisotropy =     8.5682
XX=    25.8776   YX=    -0.1763   ZX=    -0.4479
XY=     0.4320   YY=    33.8286   ZY=     3.0648
XZ=    -0.8319   YZ=     3.3993   ZZ=    31.0198
Eigenvalues:    25.7553    29.0166    35.9541
  22  H    Isotropic =    29.6526   Anisotropy =     6.1968
XX=    32.8646   YX=    -1.0834   ZX=    -2.0777
XY=    -1.1939   YY=    29.7721   ZY=    -0.1725
XZ=    -2.4440   YZ=    -0.9797   ZZ=    26.3211
Eigenvalues:    25.4296    29.7444    33.7838
```

```
  23  H    Isotropic =    29.9864   Anisotropy =     5.4068
XX=    32.2849   YX=    -0.3909   ZX=     2.8113
XY=    -0.7942   YY=    26.4791   ZY=    -0.4593
XZ=     0.6901   YZ=     0.8897   ZZ=    31.1951
Eigenvalues:    26.3839    29.9842    33.5909
  24  H    Isotropic =    29.9939   Anisotropy =     9.8584
XX=    27.8603   YX=     1.4606   ZX=    -2.6284
XY=     0.9409   YY=    27.1768   ZY=    -1.8126
XZ=    -3.9922   YZ=    -0.9334   ZZ=    34.9446
Eigenvalues:    26.0852    27.3303    36.5662
  25  H    Isotropic =    29.2603   Anisotropy =     7.1081
XX=    28.6932   YX=    -2.3174   ZX=     0.1020
XY=    -1.9893   YY=    32.4964   ZY=    -1.2923
XZ=    -0.7176   YZ=    -3.2685   ZZ=    26.5913
Eigenvalues:    25.4595    28.3223    33.9990
  26  H    Isotropic =    27.7551   Anisotropy =     5.6132
XX=    28.2052   YX=    -0.5799   ZX=    -0.3442
XY=     0.3061   YY=    28.5567   ZY=     2.9689
XZ=     1.2346   YZ=     4.6784   ZZ=    26.5035
Eigenvalues:    23.5302    28.2379    31.4972
  27  H    Isotropic =    28.1052   Anisotropy =     3.6440
XX=    28.5993   YX=     0.2838   ZX=    -2.4191
XY=     0.1410   YY=    25.9512   ZY=    -1.4553
XZ=     1.3639   YZ=    -1.8069   ZZ=    29.7651
Eigenvalues:    25.3487    28.4324    30.5345
  28  H    Isotropic =    30.6420   Anisotropy =     8.7618
XX=    27.1050   YX=    -0.0221   ZX=     0.1977
XY=     0.7086   YY=    36.0576   ZY=     2.3719
XZ=     0.3017   YZ=     1.1793   ZZ=    28.7633
Eigenvalues:    27.0673    28.3755    36.4832
  29  H    Isotropic =    30.6961   Anisotropy =     9.5784
XX=    27.9822   YX=     0.8626   ZX=    -1.8173
XY=     1.4786   YY=    31.6523   ZY=    -4.7275
XZ=    -2.1415   YZ=    -4.1773   ZZ=    32.4540
Eigenvalues:    27.0392    27.9675    37.0817
  30  H    Isotropic =    30.1421   Anisotropy =     8.1116
XX=    32.6854   YX=    -2.1441   ZX=     2.6189
XY=    -2.4646   YY=    31.4907   ZY=    -1.6467
XZ=     2.8598   YZ=    -1.6220   ZZ=    26.2502
Eigenvalues:    25.1427    29.7339    35.5498
  31  H    Isotropic =    25.7545   Anisotropy =     6.7613
XX=    28.7785   YX=     2.2519   ZX=     1.2569
XY=     1.8662   YY=    26.3084   ZY=     1.1046
XZ=     1.1676   YZ=     1.1076   ZZ=    22.1766
Eigenvalues:    21.8214    25.1801    30.2621
  32  H    Isotropic =    25.3315   Anisotropy =     8.0395
XX=    30.2532   YX=    -1.5836   ZX=     0.9914
XY=    -1.4127   YY=    24.4247   ZY=     0.1738
XZ=     0.8022   YZ=     0.0922   ZZ=    21.3167
Eigenvalues:    21.2012    24.1021    30.6912
  33  H    Isotropic =    29.4287   Anisotropy =     8.6494
XX=    30.6986   YX=    -1.4165   ZX=     3.8230
```

```
XY=    -0.5802   YY=    28.2006   ZY=    -2.0595
XZ=     4.8731   YZ=    -2.6002   ZZ=    29.3870
Eigenvalues:    25.1475    27.9437    35.1950
  34  H    Isotropic =    29.4476   Anisotropy =     8.8350
XX=    33.2445   YX=    -1.2540   ZX=    -3.2693
XY=     0.0745   YY=    27.1968   ZY=     1.9477
XZ=    -3.9670   YZ=     2.1523   ZZ=    27.9014
Eigenvalues:    24.9028    28.1024    35.3375
  35  H    Isotropic =    29.9225   Anisotropy =     7.6309
XX=    31.7978   YX=     3.5214   ZX=     1.4759
XY=     0.9177   YY=    32.9091   ZY=     1.2598
XZ=     1.0574   YZ=     1.6183   ZZ=    25.0604
Eigenvalues:    24.6900    30.0676    35.0097
  36  H    Isotropic =    28.1422   Anisotropy =    14.9614
XX=    30.9962   YX=    -4.6447   ZX=     0.6275
XY=    -6.5293   YY=    33.6095   ZY=     1.5742
XZ=     0.3032   YZ=     2.1525   ZZ=    19.8207
Eigenvalues:    19.4226    26.8875    38.1164
  37  H    Isotropic =    26.5762   Anisotropy =     6.2223
XX=    28.5282   YX=     0.3618   ZX=    -1.8763
XY=    -1.2541   YY=    25.3908   ZY=     0.4686
XZ=    -4.5886   YZ=     0.0335   ZZ=    25.8098
Eigenvalues:    23.6615    25.3428    30.7244
  38  H    Isotropic =    26.5006   Anisotropy =     8.3303
XX=    30.1390   YX=    -1.3820   ZX=    -5.0258
XY=     1.1349   YY=    24.3201   ZY=    -0.2719
XZ=    -2.3029   YZ=    -0.1453   ZZ=    25.0428
Eigenvalues:    23.0804    24.3673    32.0541
  39  H    Isotropic =    28.9533   Anisotropy =     4.3110
XX=    26.8973   YX=     2.5432   ZX=     1.3316
XY=     2.2635   YY=    28.3919   ZY=    -0.1698
XZ=     0.5911   YZ=     0.0242   ZZ=    31.5706
Eigenvalues:    25.0249    30.0077    31.8273
  40  H    Isotropic =    29.8154   Anisotropy =     7.0417
XX=    30.6894   YX=    -0.5598   ZX=     0.6146
XY=    -1.9974   YY=    33.8720   ZY=     1.7423
XZ=    -0.4479   YZ=     1.1562   ZZ=    24.8848
Eigenvalues:    24.6435    30.2929    34.5099
  41  H    Isotropic =    29.7841   Anisotropy =     8.6785
XX=    32.2841   YX=     3.0925   ZX=    -0.9696
XY=     4.9175   YY=    30.5743   ZY=     1.5341
XZ=     0.1972   YZ=     1.4334   ZZ=    26.4940
Eigenvalues:    25.4301    28.3525    35.5698
  42  H    Isotropic =    29.8777   Anisotropy =    18.8943
XX=    32.1514   YX=     4.4699   ZX=    -5.8041
XY=     4.8799   YY=    25.0704   ZY=    -7.0519
XZ=    -5.7255   YZ=    -8.1822   ZZ=    32.4113
Eigenvalues:    20.1948    26.9644    42.4739
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 71.52 | 81.35 | 94.56 | 121.71 | 152.20 | 171.97 |
| intensities | 0.30 | 0.34 | 1.46 | 0.75 | 2.79 | 0.84 |
| reduc. mass | 1.80 | 1.17 | 1.00 | 1.43 | 2.91 | 1.02 |
| force const | 0.01 | 0.00 | 0.01 | 0.01 | 0.04 | 0.02 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 214.66 | 221.35 | 242.76 | 250.67 | 263.19 | 274.79 |
| intensities | 1.66 | 0.80 | 3.71 | 1.33 | 5.75 | 4.72 |
| reduc. mass | 0.88 | 0.81 | 1.06 | 0.51 | 1.14 | 3.83 |
| force const | 0.02 | 0.02 | 0.04 | 0.02 | 0.05 | 0.17 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 292.23 | 297.70 | 321.76 | 328.14 | 332.18 | 351.25 |
| intensities | 1.30 | 0.98 | 0.27 | 1.15 | 2.84 | 5.88 |
| reduc. mass | 0.21 | 0.34 | 0.67 | 0.35 | 0.55 | 0.60 |
| force const | 0.01 | 0.02 | 0.04 | 0.02 | 0.04 | 0.04 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| frequencies | 362.71 | 393.63 | 433.60 | 443.39 | 467.18 | 496.98 |
| intensities | 0.46 | 5.69 | 2.09 | 34.08 | 39.72 | 30.75 |
| reduc. mass | 0.72 | 0.55 | 0.80 | 0.46 | 0.47 | 0.59 |
| force const | 0.06 | 0.05 | 0.09 | 0.05 | 0.06 | 0.09 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 510.88 | 522.90 | 526.44 | 568.45 | 588.48 | 600.67 |
| intensities | 7.00 | 17.84 | 7.41 | 12.23 | 3.75 | 8.86 |
| reduc. mass | 0.67 | 2.70 | 0.56 | 0.73 | 1.18 | 1.97 |
| force const | 0.10 | 0.43 | 0.09 | 0.14 | 0.24 | 0.42 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 627.49 | 647.24 | 676.52 | 687.29 | 718.29 | 732.73 |
| intensities | 45.07 | 0.88 | 25.88 | 2.86 | 1.76 | 4.30 |
| reduc. mass | 0.57 | 0.90 | 0.85 | 1.29 | 0.37 | 0.58 |
| force const | 0.13 | 0.22 | 0.23 | 0.36 | 0.11 | 0.18 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 756.07 | 803.93 | 825.66 | 842.40 | 867.45 | 887.80 |
| intensities | 0.34 | 3.80 | 2.97 | 0.88 | 37.38 | 12.09 |
| reduc. mass | 2.18 | 0.86 | 0.76 | 2.42 | 0.56 | 0.97 |
| force const | 0.73 | 0.33 | 0.31 | 1.01 | 0.25 | 0.45 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 906.59 | 933.48 | 951.21 | 990.49 | 1005.64 | 1010.73 |

| | | | | | | |
|---|---|---|---|---|---|---|
| intensities | 6.76 | 1.86 | 14.47 | 0.54 | 4.09 | 23.29 |
| reduc. mass | 0.63 | 1.47 | 0.33 | 0.37 | 0.35 | 0.27 |
| force const | 0.30 | 0.76 | 0.18 | 0.21 | 0.21 | 0.16 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1030.34 | 1035.86 | 1053.27 | 1067.27 | 1086.07 | 1099.70 |
| intensities | 29.40 | 8.54 | 1.46 | 48.52 | 69.75 | 2.34 |
| reduc. mass | 0.31 | 0.28 | 0.27 | 0.61 | 0.46 | 0.66 |
| force const | 0.19 | 0.18 | 0.17 | 0.41 | 0.32 | 0.47 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1103.14 | 1111.59 | 1144.87 | 1180.81 | 1186.20 | 1211.26 |
| intensities | 15.67 | 47.06 | 10.77 | 39.89 | 4.62 | 62.66 |
| reduc. mass | 0.39 | 1.02 | 0.36 | 0.83 | 0.51 | 0.35 |
| force const | 0.28 | 0.74 | 0.27 | 0.68 | 0.42 | 0.30 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1231.66 | 1239.85 | 1250.19 | 1258.94 | 1314.86 | 1329.14 |
| intensities | 11.91 | 31.84 | 88.95 | 3.64 | 12.07 | 148.06 |
| reduc. mass | 0.53 | 0.38 | 0.86 | 0.33 | 1.84 | 0.38 |
| force const | 0.47 | 0.34 | 0.79 | 0.31 | 1.88 | 0.40 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1335.99 | 1376.61 | 1406.99 | 1435.81 | 1458.39 | 1479.62 |
| intensities | 21.42 | 34.68 | 40.36 | 731.75 | 67.98 | 35.78 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.62 | 0.50 | 0.42 | 0.63 | 0.49 | 0.80 |
| force const | 0.65 | 0.56 | 0.49 | 0.77 | 0.62 | 1.03 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1484.70 | 1507.78 | 1515.79 | 1523.19 | 1526.13 | 1551.48 |
| intensities | 34.95 | 0.64 | 139.98 | 43.49 | 39.08 | 4.70 |
| reduc. mass | 0.88 | 0.72 | 1.57 | 0.46 | 2.78 | 0.71 |
| force const | 1.15 | 0.97 | 2.12 | 0.63 | 3.82 | 1.01 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1566.18 | 1577.91 | 1580.14 | 1605.08 | 1626.73 | 1630.18 |
| intensities | 10.45 | 51.20 | 10.03 | 33.90 | 0.86 | 149.49 |
| reduc. mass | 0.98 | 1.25 | 0.62 | 0.68 | 0.88 | 0.41 |
| force const | 1.42 | 1.84 | 0.91 | 1.04 | 1.37 | 0.65 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1643.35 | 1653.10 | 1657.19 | 1660.63 | 1662.54 | 1664.08 |
| intensities | 12.17 | 16.73 | 27.25 | 11.02 | 24.78 | 8.66 |
| reduc. mass | 0.61 | 0.20 | 0.49 | 0.36 | 0.17 | 0.27 |
| force const | 0.98 | 0.33 | 0.80 | 0.58 | 0.28 | 0.44 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1666.33 | 1671.39 | 1679.05 | 1679.79 | 1686.08 | 1799.71 |
| intensities | 26.46 | 40.27 | 4.37 | 3.70 | 39.65 | 1294.97 |
| reduc. mass | 0.26 | 0.24 | 0.37 | 0.38 | 1.38 | 1.40 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 0.43 | 0.39 | 0.61 | 0.64 | 2.32 | 2.67 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1835.21 | 1890.45 | 3022.95 | 3027.75 | 3029.50 | 3058.93 |
| intensities | 291.59 | 19.56 | 274.35 | 668.08 | 537.26 | 366.93 |
| reduc. mass | 1.30 | 0.84 | 0.33 | 0.18 | 0.18 | 0.44 |
| force const | 2.58 | 1.78 | 1.78 | 0.98 | 0.98 | 2.42 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3067.30 | 3072.14 | 3089.37 | 3100.41 | 3108.26 | 3125.58 |
| intensities | 399.32 | 119.87 | 336.70 | 589.37 | 217.80 | 402.01 |
| reduc. mass | 0.37 | 0.78 | 0.92 | 0.46 | 0.87 | 0.41 |
| force const | 2.04 | 4.36 | 5.17 | 2.59 | 4.95 | 2.38 |

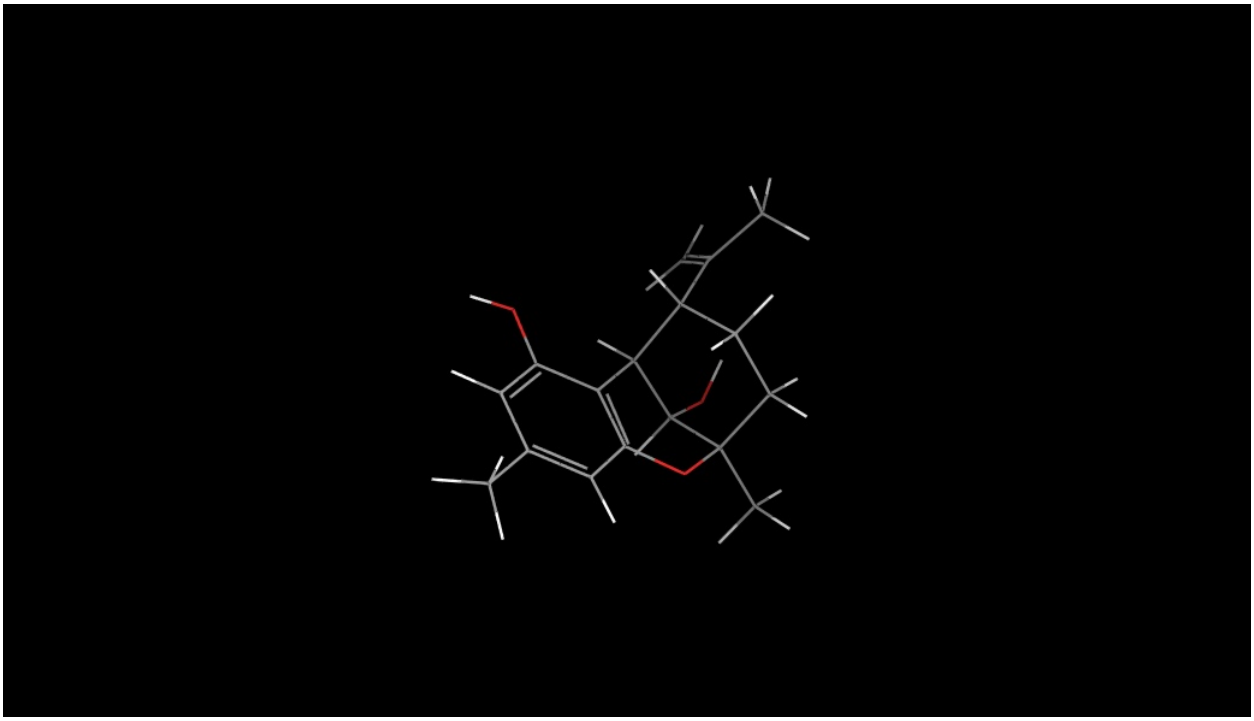
| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3131.00 | 3134.26 | 3135.30 | 3137.62 | 3144.44 | 3147.39 |
| intensities | 258.96 | 378.94 | 354.00 | 407.92 | 366.59 | 382.46 |
| reduc. mass | 0.46 | 0.33 | 0.40 | 0.84 | 0.54 | 0.51 |
| force const | 2.63 | 1.91 | 2.33 | 4.84 | 3.14 | 3.00 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3148.30 | 3153.40 | 3156.96 | 3203.76 | 3823.46 | 3860.28 |
| intensities | 482.35 | 300.81 | 285.25 | 368.42 | 27.31 | 34.34 |
| reduc. mass | 0.55 | 0.57 | 0.86 | 0.56 | 0.95 | 0.95 |
| force const | 3.22 | 3.35 | 5.07 | 3.40 | 8.15 | 8.32 |

Number of imaginary frequencies: 0

Conformation 4

Boltzmann Population = 1.1% (relative energy = 2.28 kcal/mol)



Geometries and Energy Method: M06-2X-D3/6-31G(d,p)

NMR Method: mPW1PW91/6-311+G(2d,p)

Thermodynamic properties for P = 1.00 atm, calculated at 1 temperatures

T = 298.15 K, P = 1.00 atm

Total internal energy, Utot(SCFE + ZPE + U): -885.983272 hartrees

Total enthalpy, Htot (Utot + pV): -885.982328 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -886.042720 hartrees

Optimized Geometry:

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 6 | 0 | -1.443800 | -2.006400 | 4.716000 |
| 2 | 6 | 0 | -1.138000 | -1.863600 | 3.224100 |
| 3 | 6 | 0 | -2.366500 | -1.405100 | 2.408500 |

| | | | | | |
|---|---|---|---|---|---|
| 4 | 6 | 0 | -2.976600 | -0.142600 | 3.077400 |
| 5 | 6 | 0 | -3.320500 | -0.342100 | 4.562600 |
| 6 | 6 | 0 | -2.032400 | -0.720900 | 5.313600 |
| 7 | 6 | 0 | -2.285900 | -0.864500 | 6.803500 |
| 8 | 6 | 0 | -3.349200 | -2.527400 | 2.083300 |
| 9 | 6 | 0 | -1.964900 | 0.977600 | 3.040500 |
| 10 | 6 | 0 | -1.078400 | 1.159100 | 4.103400 |
| 11 | 8 | 0 | -1.067800 | 0.346400 | 5.194400 |
| 12 | 6 | 0 | -1.861300 | 1.848400 | 1.952500 |
| 13 | 6 | 0 | -0.927100 | 2.878100 | 1.930900 |
| 14 | 6 | 0 | -0.056800 | 3.052900 | 3.010400 |
| 15 | 6 | 0 | -0.136100 | 2.190600 | 4.096300 |
| 16 | 6 | 0 | 0.980900 | 4.145900 | 2.974200 |
| 17 | 8 | 0 | -2.721800 | 1.623400 | 0.917300 |
| 18 | 6 | 0 | -4.678100 | -2.378900 | 2.053200 |
| 19 | 6 | 0 | -2.731600 | -3.837200 | 1.658000 |
| 20 | 8 | 0 | -4.343900 | -1.272900 | 4.831400 |
| 21 | 1 | 0 | -0.534300 | -2.264600 | 5.268300 |
| 22 | 1 | 0 | -2.162900 | -2.819200 | 4.887300 |
| 23 | 1 | 0 | -0.344500 | -1.120900 | 3.098000 |
| 24 | 1 | 0 | -0.737500 | -2.800700 | 2.829500 |
| 25 | 1 | 0 | -1.991300 | -1.078800 | 1.426500 |
| 26 | 1 | 0 | -3.865700 | 0.176900 | 2.526500 |
| 27 | 1 | 0 | -3.672500 | 0.616700 | 4.963400 |
| 28 | 1 | 0 | -1.352000 | -1.101300 | 7.320300 |
| 29 | 1 | 0 | -2.677600 | 0.073500 | 7.205700 |
| 30 | 1 | 0 | -3.015600 | -1.655200 | 6.982700 |
| 31 | 1 | 0 | -0.873200 | 3.544200 | 1.072600 |
| 32 | 1 | 0 | 0.524900 | 2.293200 | 4.950100 |
| 33 | 1 | 0 | 0.609500 | 5.027100 | 2.445200 |
| 34 | 1 | 0 | 1.270500 | 4.447900 | 3.982900 |
| 35 | 1 | 0 | 1.883900 | 3.806100 | 2.456800 |
| 36 | 1 | 0 | -2.577300 | 2.290500 | 0.237300 |
| 37 | 1 | 0 | -5.316300 | -3.195300 | 1.729000 |
| 38 | 1 | 0 | -5.176500 | -1.460100 | 2.340900 |
| 39 | 1 | 0 | -2.264100 | -4.353600 | 2.503100 |
| 40 | 1 | 0 | -1.946300 | -3.672600 | 0.911600 |
| 41 | 1 | 0 | -3.482700 | -4.502700 | 1.228600 |
| 42 | 1 | 0 | -4.241800 | -2.029000 | 4.239400 |

---

SCF GIAO Magnetic shielding tensor (ppm):
1 C Isotropic = 155.4920 Anisotropy = 26.9860
XX= 148.9628 YX= 4.7711 ZX= -8.0840
XY= 4.3788 YY= 160.0291 ZY= -5.6471
XZ= -12.9033 YZ= -14.5199 ZZ= 157.4842
Eigenvalues: 141.6420 151.3513 173.4827
2 C Isotropic = 164.6721 Anisotropy = 16.0160
XX= 157.3596 YX= -0.3521 ZX= -2.4693

```
XY=     0.6313   YY=   174.1885   ZY=     4.3621
XZ=    -2.8816   YZ=     3.2897   ZZ=   162.4682
Eigenvalues:   156.0537   162.6131   175.3494
   3  C    Isotropic =   140.7349   Anisotropy =    30.1772
XX=   158.8250   YX=     4.3255   ZX=    -0.8354
XY=     3.8651   YY=   138.8942   ZY=    -7.9000
XZ=   -11.2420   YZ=     0.5563   ZZ=   124.4856
Eigenvalues:   122.8974   138.4543   160.8531
   4  C    Isotropic =   152.3693   Anisotropy =    19.2733
XX=   151.3940   YX=     1.2376   ZX=    -2.0762
XY=    -6.6425   YY=   144.4085   ZY=   -12.0656
XZ=     2.0713   YZ=    -5.7516   ZZ=   161.3055
Eigenvalues:   140.0342   151.8557   165.2182
   5  C    Isotropic =   111.8397   Anisotropy =    43.8982
XX=   140.5089   YX=     6.5530   ZX=    10.7980
XY=    -0.5615   YY=   102.2793   ZY=    -1.3851
XZ=    -2.3364   YZ=     0.6481   ZZ=    92.7308
Eigenvalues:    92.3186   102.0952   141.1051
   6  C    Isotropic =   107.9128   Anisotropy =    66.0938
XX=   145.3636   YX=    -4.1959   ZX=    17.4170
XY=     5.1868   YY=    85.2028   ZY=    -6.1711
XZ=    21.8424   YZ=    -8.5987   ZZ=    93.1721
Eigenvalues:    78.6859    93.0773   151.9753
   7  C    Isotropic =   160.3708   Anisotropy =    41.4624
XX=   146.7106   YX=    -6.2314   ZX=    -0.8305
XY=    -5.9307   YY=   181.3815   ZY=   -16.1145
XZ=    -1.6087   YZ=   -12.5637   ZZ=   153.0203
Eigenvalues:   143.0753   150.0247   188.0124
   8  C    Isotropic =    27.6104   Anisotropy =   188.8960
XX=   -40.6790   YX=   -65.6497   ZX=    45.4978
XY=   -71.0341   YY=   128.8668   ZY=     8.4391
XZ=    48.6656   YZ=     5.4743   ZZ=    -5.3565
Eigenvalues:   -90.5216    19.8117   153.5411
   9  C    Isotropic =    72.9853   Anisotropy =   127.7962
XX=    28.0446   YX=     4.1316   ZX=   -28.0798
XY=     5.2389   YY=    46.4003   ZY=   -33.8013
XZ=   -19.8390   YZ=   -28.7735   ZZ=   144.5109
Eigenvalues:    23.1669    37.6061   158.1827
  10  C    Isotropic =    24.2315   Anisotropy =   139.0804
XX=   -10.1831   YX=    41.2969   ZX=   -13.7261
XY=    48.4109   YY=   -19.5738   ZY=   -32.3747
XZ=   -14.5005   YZ=   -36.6888   ZZ=   102.4512
Eigenvalues:   -61.7078    17.4504   116.9517
  11  O    Isotropic =   171.5023   Anisotropy =    68.3043
XX=   122.8886   YX=     2.6832   ZX=   -21.4704
XY=   -27.4572   YY=   190.0801   ZY=    -7.2861
XZ=   -16.7355   YZ=   -32.0585   ZZ=   201.5382
Eigenvalues:   114.7417   182.7267   217.0385
  12  C    Isotropic =    29.4368   Anisotropy =   130.7373
XX=    21.3392   YX=   -24.1879   ZX=   -26.0195
XY=   -15.2703   YY=   -34.5768   ZY=   -42.5520
XZ=   -21.0570   YZ=   -40.8916   ZZ=   101.5480
```

```
Eigenvalues:   -54.9866    26.7020   116.5950
  13  C    Isotropic =    80.3721   Anisotropy =    98.5397
XX=    65.1044   YX=    39.5627   ZX=    -6.7154
XY=    47.0847   YY=    39.1203   ZY=   -20.0031
XZ=   -11.0694   YZ=   -22.8855   ZZ=   136.8916
Eigenvalues:     5.7664    89.2846   146.0652
  14  C    Isotropic =    43.2983   Anisotropy =   193.4997
XX=   -44.9028   YX=    -1.5187   ZX=   -46.6422
XY=    -2.3719   YY=    22.4891   ZY=   -42.3684
XZ=   -40.2433   YZ=   -40.6951   ZZ=   152.3085
Eigenvalues:   -55.5975    13.1942   172.2981
  15  C    Isotropic =    75.2934   Anisotropy =   115.9933
XX=    69.6783   YX=   -19.2119   ZX=   -23.2852
XY=   -22.9123   YY=    21.6565   ZY=   -41.5129
XZ=   -31.6568   YZ=   -39.6058   ZZ=   134.5453
Eigenvalues:    -2.9708    76.2287   152.6222
  16  C    Isotropic =   164.3762   Anisotropy =    40.9340
XX=   189.4307   YX=     4.1558   ZX=     5.1261
XY=     0.9342   YY=   157.2259   ZY=     3.8572
XZ=    13.2823   YZ=     5.4963   ZZ=   146.4719
Eigenvalues:   143.3663   158.0967   191.6655
  17  O    Isotropic =   216.0244   Anisotropy =    48.9963
XX=   179.3156   YX=    10.8728   ZX=    -6.5440
XY=    35.7356   YY=   230.7464   ZY=     7.0507
XZ=    -2.3105   YZ=    16.4304   ZZ=   238.0111
Eigenvalues:   169.2923   230.0923   248.6886
  18  C    Isotropic =    67.8716   Anisotropy =   131.1258
XX=    -1.9973   YX=   -52.9785   ZX=    44.2069
XY=   -47.3431   YY=   139.1526   ZY=    11.7094
XZ=    43.3225   YZ=     9.6723   ZZ=    66.4595
Eigenvalues:   -37.4547    85.7807   155.2888
  19  C    Isotropic =   161.2365   Anisotropy =    33.7588
XX=   163.5989   YX=     7.2060   ZX=   -14.6425
XY=     8.1067   YY=   149.5526   ZY=    -7.0101
XZ=   -11.1695   YZ=    -7.9785   ZZ=   170.5579
Eigenvalues:   145.9891   153.9779   183.7423
  20  O    Isotropic =   267.7643   Anisotropy =    70.8291
XX=   248.8809   YX=    17.1457   ZX=    -9.5893
XY=    16.4298   YY=   283.1452   ZY=   -28.0005
XZ=   -35.3135   YZ=   -23.6900   ZZ=   271.2669
Eigenvalues:   234.9715   253.3378   314.9837
  21  H    Isotropic =    30.3465   Anisotropy =     8.9291
XX=    25.8051   YX=    -0.5845   ZX=    -1.3185
XY=     0.1143   YY=    33.6504   ZY=     3.2667
XZ=    -1.3742   YZ=     3.6035   ZZ=    31.5841
Eigenvalues:    25.4655    29.2749    36.2992
  22  H    Isotropic =    30.0607   Anisotropy =     5.7597
XX=    33.1212   YX=    -1.3278   ZX=    -1.4788
XY=    -1.2683   YY=    29.7527   ZY=    -0.3488
XZ=    -1.8759   YZ=    -0.3723   ZZ=    27.3080
Eigenvalues:    26.6952    29.5863    33.9005
  23  H    Isotropic =    29.9515   Anisotropy =     4.9921
```

```
XX=    32.3878   YX=    -0.3397   ZX=     2.5810
XY=     0.2010   YY=    26.2708   ZY=    -0.9841
XZ=     0.1241   YZ=     0.2417   ZZ=    31.1959
Eigenvalues:    26.2428    30.3321    33.2796
  24  H    Isotropic =    30.0438   Anisotropy =     9.4946
XX=    28.2223   YX=     3.0541   ZX=    -2.8384
XY=     3.1162   YY=    28.3805   ZY=    -1.4474
XZ=    -4.2540   YZ=    -1.8306   ZZ=    33.5288
Eigenvalues:    24.9180    28.8399    36.3736
  25  H    Isotropic =    29.1899   Anisotropy =     7.0163
XX=    29.5824   YX=    -2.3135   ZX=     0.0038
XY=    -2.3281   YY=    32.3748   ZY=    -1.6044
XZ=    -2.6766   YZ=    -2.5619   ZZ=    25.6126
Eigenvalues:    24.2725    29.4298    33.8675
  26  H    Isotropic =    27.5273   Anisotropy =     6.6930
XX=    27.7193   YX=    -1.4510   ZX=    -0.4300
XY=    -1.5361   YY=    27.3233   ZY=     4.0317
XZ=     1.7220   YZ=     4.9135   ZZ=    27.5394
Eigenvalues:    22.5108    28.0818    31.9893
  27  H    Isotropic =    28.0474   Anisotropy =     3.4241
XX=    28.6697   YX=     0.2744   ZX=    -2.2009
XY=    -0.1923   YY=    25.9550   ZY=    -1.5807
XZ=     1.5847   YZ=    -2.0399   ZZ=    29.5174
Eigenvalues:    25.1947    28.6173    30.3301
  28  H    Isotropic =    30.6887   Anisotropy =     8.8114
XX=    27.1678   YX=     0.1698   ZX=     0.2087
XY=     0.8537   YY=    35.6493   ZY=     3.1133
XZ=     0.3673   YZ=     1.9429   ZZ=    29.2489
Eigenvalues:    27.1236    28.3795    36.5630
  29  H    Isotropic =    30.7029   Anisotropy =     9.4818
XX=    28.2535   YX=     1.3234   ZX=    -2.0107
XY=     2.0606   YY=    32.4615   ZY=    -4.5089
XZ=    -2.2387   YZ=    -3.9817   ZZ=    31.3938
Eigenvalues:    27.0771    28.0076    37.0241
  30  H    Isotropic =    30.1110   Anisotropy =     8.1887
XX=    32.2168   YX=    -2.4437   ZX=     2.7182
XY=    -2.7310   YY=    31.8923   ZY=    -1.2855
XZ=     2.9005   YZ=    -1.2369   ZZ=    26.2238
Eigenvalues:    25.1043    29.6585    35.5701
  31  H    Isotropic =    25.7749   Anisotropy =     6.5311
XX=    28.7478   YX=     1.7572   ZX=     1.6292
XY=     1.5134   YY=    25.8104   ZY=     1.6647
XZ=     1.4741   YZ=     1.9787   ZZ=    22.7664
Eigenvalues:    21.8295    25.3662    30.1289
  32  H    Isotropic =    25.3063   Anisotropy =     8.2557
XX=    30.2461   YX=    -1.8522   ZX=     1.0889
XY=    -1.5818   YY=    24.3973   ZY=     0.3871
XZ=     1.0015   YZ=    -0.0231   ZZ=    21.2754
Eigenvalues:    21.1076    24.0012    30.8101
  33  H    Isotropic =    29.7542   Anisotropy =     8.3404
XX=    33.6862   YX=    -2.9161   ZX=    -2.1292
XY=    -0.8490   YY=    28.7653   ZY=     2.9504
```

```
XZ=    -1.8494   YZ=     2.7563   ZZ=    26.8112
Eigenvalues:    24.7369    29.2113    35.3145
  34  H    Isotropic =    29.7350   Anisotropy =     7.8093
XX=    32.1367   YX=     3.7439   ZX=     0.7273
XY=     1.5552   YY=    32.4259   ZY=    -0.1111
XZ=    -0.0089   YZ=     0.1349   ZZ=    24.6424
Eigenvalues:    24.6233    29.6405    34.9412
  35  H    Isotropic =    29.3575   Anisotropy =     8.8574
XX=    29.8059   YX=    -0.7230   ZX=     3.5991
XY=    -0.9260   YY=    26.5999   ZY=    -1.2162
XZ=     4.7738   YZ=    -1.1383   ZZ=    31.6668
Eigenvalues:    26.3035    26.5067    35.2624
  36  H    Isotropic =    28.1767   Anisotropy =    14.9798
XX=    30.7272   YX=    -4.6871   ZX=     0.3318
XY=    -6.7367   YY=    33.1669   ZY=     2.9852
XZ=    -0.2660   YZ=     3.5984   ZZ=    20.6359
Eigenvalues:    19.6057    26.7611    38.1632
  37  H    Isotropic =    26.2992   Anisotropy =     5.4914
XX=    24.9289   YX=     0.9923   ZX=     0.6904
XY=     1.9072   YY=    26.1759   ZY=     1.2340
XZ=     3.4492   YZ=     1.7827   ZZ=    27.7927
Eigenvalues:    23.6497    25.2877    29.9601
  38  H    Isotropic =    25.7522   Anisotropy =     7.4919
XX=    25.3156   YX=     2.6039   ZX=     5.4387
XY=     1.6324   YY=    26.2881   ZY=     2.3736
XZ=     1.3930   YZ=     1.5043   ZZ=    25.6528
Eigenvalues:    22.0514    24.4584    30.7468
  39  H    Isotropic =    29.7372   Anisotropy =     6.2680
XX=    30.3704   YX=     0.0250   ZX=    -3.7906
XY=     0.5199   YY=    29.9159   ZY=     2.7570
XZ=    -3.3729   YZ=     2.4668   ZZ=    28.9255
Eigenvalues:    24.9693    30.3265    33.9159
  40  H    Isotropic =    30.1442   Anisotropy =     7.8644
XX=    28.9495   YX=     1.0088   ZX=    -0.3094
XY=     1.0643   YY=    29.8065   ZY=    -4.9145
XZ=     0.5047   YZ=    -4.0790   ZZ=    31.6766
Eigenvalues:    25.8999    29.1455    35.3872
  41  H    Isotropic =    29.8861   Anisotropy =     8.3948
XX=    32.7892   YX=     4.1995   ZX=     0.3454
XY=     4.3937   YY=    28.2856   ZY=     0.2158
XZ=    -1.9563   YZ=    -0.6685   ZZ=    28.5834
Eigenvalues:    25.6690    28.5066    35.4826
  42  H    Isotropic =    29.8911   Anisotropy =    19.6497
XX=    32.8488   YX=     7.1262   ZX=    -2.4352
XY=     8.0791   YY=    30.5681   ZY=    -7.9004
XZ=    -3.2158   YZ=    -8.5735   ZZ=    26.2564
Eigenvalues:    19.3242    27.3582    42.9909
```

Number of frequencies: 120

harmonic frequencies in cm**-1, reduced masses in amu,

force constants in mDyne/A, and

normal modes in cartesian coordinates: 120

IR intensities in km/mol

| vibration # | 1 | 2 | 3 | 4 | 5 | 6 |
|---|---|---|---|---|---|---|
| frequencies | 71.00 | 82.16 | 90.56 | 134.54 | 153.97 | 180.60 |
| intensities | 0.63 | 0.07 | 1.07 | 1.54 | 0.51 | 1.69 |
| reduc. mass | 1.84 | 1.60 | 0.75 | 2.22 | 1.49 | 0.88 |
| force const | 0.01 | 0.01 | 0.00 | 0.02 | 0.02 | 0.02 |

| vibration # | 7 | 8 | 9 | 10 | 11 | 12 |
|---|---|---|---|---|---|---|
| frequencies | 214.54 | 217.75 | 236.95 | 254.16 | 264.39 | 288.66 |
| intensities | 0.02 | 2.49 | 2.17 | 0.84 | 5.35 | 1.10 |
| reduc. mass | 0.63 | 0.82 | 0.90 | 0.87 | 0.91 | 0.93 |
| force const | 0.02 | 0.02 | 0.03 | 0.03 | 0.04 | 0.05 |

| vibration # | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|
| frequencies | 296.01 | 304.09 | 319.27 | 326.66 | 336.28 | 347.96 |
| intensities | 0.57 | 0.89 | 1.51 | 0.78 | 2.07 | 3.16 |
| reduc. mass | 2.78 | 0.23 | 0.54 | 0.40 | 0.49 | 0.57 |
| force const | 0.14 | 0.01 | 0.03 | 0.03 | 0.03 | 0.04 |

| vibration # | 19 | 20 | 21 | 22 | 23 | 24 |
|---|---|---|---|---|---|---|
| frequencies | 376.13 | 423.70 | 424.57 | 461.57 | 484.75 | 490.67 |
| intensities | 0.10 | 9.84 | 5.17 | 2.28 | 9.81 | 0.44 |

| | | | | | | |
|---|---|---|---|---|---|---|
| reduc. mass | 0.78 | 0.56 | 1.00 | 1.16 | 0.71 | 0.67 |
| force const | 0.06 | 0.06 | 0.11 | 0.15 | 0.10 | 0.09 |

| vibration # | 25 | 26 | 27 | 28 | 29 | 30 |
|---|---|---|---|---|---|---|
| frequencies | 521.40 | 533.17 | 557.82 | 564.75 | 600.39 | 612.98 |
| intensities | 10.87 | 19.06 | 8.35 | 2.10 | 10.68 | 6.85 |
| reduc. mass | 2.50 | 0.58 | 0.52 | 0.50 | 1.31 | 0.96 |
| force const | 0.40 | 0.10 | 0.10 | 0.09 | 0.28 | 0.21 |

| vibration # | 31 | 32 | 33 | 34 | 35 | 36 |
|---|---|---|---|---|---|---|
| frequencies | 630.54 | 660.01 | 677.46 | 697.38 | 723.39 | 730.59 |
| intensities | 23.61 | 108.07 | 10.22 | 15.86 | 3.08 | 8.93 |
| reduc. mass | 0.54 | 0.39 | 0.67 | 1.03 | 0.54 | 1.02 |
| force const | 0.13 | 0.10 | 0.18 | 0.29 | 0.17 | 0.32 |

| vibration # | 37 | 38 | 39 | 40 | 41 | 42 |
|---|---|---|---|---|---|---|
| frequencies | 745.43 | 795.84 | 827.25 | 843.81 | 868.01 | 892.35 |
| intensities | 3.58 | 2.66 | 3.97 | 0.07 | 36.43 | 3.16 |
| reduc. mass | 0.25 | 0.60 | 0.98 | 3.18 | 0.55 | 0.54 |
| force const | 0.08 | 0.22 | 0.39 | 1.34 | 0.24 | 0.25 |

| vibration # | 43 | 44 | 45 | 46 | 47 | 48 |
|---|---|---|---|---|---|---|
| frequencies | 908.50 | 933.50 | 958.66 | 992.67 | 1010.16 | 1013.65 |
| intensities | 10.36 | 3.94 | 16.78 | 2.83 | 39.22 | 5.33 |
| reduc. mass | 0.81 | 1.99 | 0.26 | 0.43 | 0.25 | 0.27 |

| | | | | | | |
|---|---|---|---|---|---|---|
| force const | 0.39 | 1.02 | 0.14 | 0.25 | 0.15 | 0.16 |

| vibration # | 49 | 50 | 51 | 52 | 53 | 54 |
|---|---|---|---|---|---|---|
| frequencies | 1025.78 | 1031.44 | 1046.98 | 1064.28 | 1087.75 | 1095.59 |
| intensities | 10.79 | 26.37 | 13.70 | 73.68 | 76.82 | 30.06 |
| reduc. mass | 0.27 | 0.41 | 0.36 | 0.42 | 0.52 | 0.49 |
| force const | 0.17 | 0.26 | 0.23 | 0.28 | 0.36 | 0.35 |

| vibration # | 55 | 56 | 57 | 58 | 59 | 60 |
|---|---|---|---|---|---|---|
| frequencies | 1105.60 | 1110.35 | 1142.24 | 1170.75 | 1184.73 | 1214.75 |
| intensities | 17.19 | 15.67 | 11.53 | 43.41 | 8.03 | 75.29 |
| reduc. mass | 0.52 | 0.68 | 0.34 | 1.34 | 0.74 | 0.43 |
| force const | 0.38 | 0.50 | 0.26 | 1.08 | 0.61 | 0.37 |

| vibration # | 61 | 62 | 63 | 64 | 65 | 66 |
|---|---|---|---|---|---|---|
| frequencies | 1223.38 | 1232.88 | 1246.93 | 1261.05 | 1313.47 | 1316.43 |
| intensities | 35.13 | 13.32 | 111.04 | 1.17 | 110.51 | 9.58 |
| reduc. mass | 0.25 | 0.31 | 0.70 | 0.31 | 0.38 | 1.49 |
| force const | 0.22 | 0.28 | 0.64 | 0.29 | 0.38 | 1.52 |

| vibration # | 67 | 68 | 69 | 70 | 71 | 72 |
|---|---|---|---|---|---|---|
| frequencies | 1339.83 | 1384.01 | 1390.50 | 1426.76 | 1447.28 | 1481.06 |
| intensities | 60.84 | 53.17 | 75.13 | 798.31 | 43.85 | 92.86 |
| reduc. mass | 1.02 | 0.57 | 0.48 | 0.73 | 0.50 | 1.10 |
| force const | 1.08 | 0.64 | 0.54 | 0.88 | 0.61 | 1.42 |

| vibration # | 73 | 74 | 75 | 76 | 77 | 78 |
|---|---|---|---|---|---|---|
| frequencies | 1494.54 | 1506.97 | 1510.33 | 1521.28 | 1532.20 | 1546.67 |
| intensities | 64.04 | 72.05 | 79.10 | 34.06 | 29.72 | 17.29 |
| reduc. mass | 0.71 | 0.96 | 0.66 | 1.90 | 0.78 | 0.79 |
| force const | 0.93 | 1.28 | 0.89 | 2.60 | 1.08 | 1.11 |

| vibration # | 79 | 80 | 81 | 82 | 83 | 84 |
|---|---|---|---|---|---|---|
| frequencies | 1565.78 | 1572.21 | 1577.61 | 1617.85 | 1627.31 | 1646.60 |
| intensities | 6.25 | 31.02 | 19.85 | 78.78 | 1.04 | 69.80 |
| reduc. mass | 0.94 | 0.75 | 0.62 | 0.40 | 0.85 | 0.44 |
| force const | 1.36 | 1.09 | 0.91 | 0.61 | 1.32 | 0.70 |

| vibration # | 85 | 86 | 87 | 88 | 89 | 90 |
|---|---|---|---|---|---|---|
| frequencies | 1651.52 | 1654.03 | 1657.29 | 1657.40 | 1660.21 | 1664.00 |
| intensities | 87.80 | 15.16 | 0.79 | 36.80 | 19.55 | 9.90 |
| reduc. mass | 0.32 | 0.30 | 0.21 | 0.24 | 0.33 | 0.24 |
| force const | 0.51 | 0.49 | 0.34 | 0.39 | 0.54 | 0.40 |

| vibration # | 91 | 92 | 93 | 94 | 95 | 96 |
|---|---|---|---|---|---|---|
| frequencies | 1669.37 | 1674.52 | 1679.51 | 1680.68 | 1706.77 | 1792.18 |
| intensities | 55.07 | 8.72 | 4.32 | 4.82 | 22.71 | 1254.21 |
| reduc. mass | 0.45 | 0.23 | 0.38 | 0.35 | 0.70 | 1.43 |
| force const | 0.73 | 0.38 | 0.63 | 0.58 | 1.21 | 2.70 |

| vibration # | 97 | 98 | 99 | 100 | 101 | 102 |
|---|---|---|---|---|---|---|
| frequencies | 1834.80 | 1890.47 | 3020.78 | 3025.02 | 3027.80 | 3050.04 |
| intensities | 292.91 | 24.97 | 275.90 | 569.81 | 688.92 | 456.05 |
| reduc. mass | 1.30 | 0.85 | 0.13 | 0.13 | 0.16 | 0.50 |
| force const | 2.58 | 1.79 | 0.70 | 0.68 | 0.85 | 2.75 |

| vibration # | 103 | 104 | 105 | 106 | 107 | 108 |
|---|---|---|---|---|---|---|
| frequencies | 3066.30 | 3072.92 | 3085.67 | 3100.91 | 3108.61 | 3121.69 |
| intensities | 243.39 | 351.44 | 354.94 | 342.03 | 240.16 | 339.73 |
| reduc. mass | 0.90 | 0.48 | 0.92 | 0.42 | 0.77 | 0.50 |
| force const | 5.00 | 2.67 | 5.14 | 2.36 | 4.37 | 2.90 |

| vibration # | 109 | 110 | 111 | 112 | 113 | 114 |
|---|---|---|---|---|---|---|
| frequencies | 3127.46 | 3132.40 | 3136.35 | 3137.50 | 3144.04 | 3146.15 |
| intensities | 406.17 | 416.27 | 637.32 | 127.14 | 405.85 | 580.42 |
| reduc. mass | 0.52 | 0.17 | 0.49 | 0.26 | 0.53 | 0.55 |
| force const | 3.02 | 0.98 | 2.82 | 1.52 | 3.11 | 3.21 |

| vibration # | 115 | 116 | 117 | 118 | 119 | 120 |
|---|---|---|---|---|---|---|
| frequencies | 3147.90 | 3153.82 | 3154.42 | 3204.18 | 3849.31 | 3855.42 |
| intensities | 337.94 | 509.74 | 115.75 | 376.95 | 61.55 | 21.63 |
| reduc. mass | 0.49 | 0.46 | 0.36 | 0.56 | 0.85 | 0.85 |
| force const | 2.85 | 2.70 | 2.13 | 3.41 | 7.44 | 7.46 |

Number of imaginary frequencies: 0